15th World Congress on Computational Mechanics

WCCM YOKOHAMA2022 APCOM

8th Asian Pacific Congress on Computational Mechanics

Yokohama Japan Virtual

Congress Vision :
Pursuing the Infinite Potential of Computational Mechanics

July 31 to August 5, 2022
(Pre-Open on July 24)

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Hosting Organizations:

International Association for Computational Mechanics (IACM)

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Supporting Organizations:

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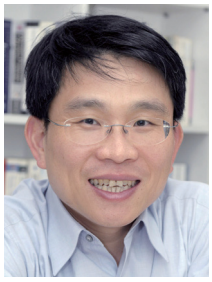

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MS0425 - Musculoskeletal Modeling Across the Lifespan: Biomechanics from Young to Aging to Aged

Organized by Geoffrey Handsfield, Justin Fernandez, Vickie Shim and Thor Besier

MS0426 - In silico clinical trials of cardiac disease

Organized by Nenad Filipovic

500 - MATERIALS BY DESIGN

MS0502 - COMPUTATIONAL MECHANICS OF SOFT MATTER

Organized by Zishun Liu

MS0503 - COMPUTATIONAL DESIGN OF ARCHITECTED MATERIALS

Organized by Julián Norato and José Guedes

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Organized by Santiago Madruga

MS0507 - Multiscale Topology Optimization

Organized by Narasimha Boddeti

MS0508 - Lessons from nature: design of bioinspired architected materials

Organized by Mohammad J. Mirzaali, Mario Milazzo, Flavia Libonati, Davide Ruffoni and Amir A. Zadpoor

600 - FLUID DYNAMICS AND TRANSPORT PHENOMENA

MS0601 - INTERFACIAL FLOW SIMULATION

Organized by Mostafa Safdari Shadloo, Amin Rahmat, Alessio Alexiadis and Mohammad Mehdi Rashidi

MS0602 - Advanced multi-physics CFD simulations in science and engineering

Organized by Takahiro Tsukahara, Kaoru Iwamoto, Koji Fukagata, Mamoru Tanahashi, Nobuyuki Oshima and Makoto Yamamoto

MS0603 - Modelling and simulation of coupled solvent transport and deformation

Organized by Jana Wilmers, Dai Okumura, Laurence Brassart and Nikolaos Bouklas

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Organized by Thomas Weinhart, Anthony R Thornton and Rudy Valette

MS0605 - COMPLEX FLUID FLOWS IN ENGINEERING: MODELING, SIMULATION AND OPTIMIZATION

Organized by Stefanie Elgeti and Marek Behr

MS0607 - Multiphase flows

Organized by Célio Fernandes, Luís Lima Ferrás and Alexandre Afonso

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Organized by Ricardo Tomás Ferreyra

MS0609 - MODELLING OF ATOMIZATION, BREAKUP AND FRAGMENTATION OF FLUIDS

Organized by Stéphane Zaleski, Junji Shinjo, Leonardo Chirco, Gretar Tryggvason and Shiyi Chen

MS0610 - Modeling and Simulation of Computational Multi-phase Flows

Organized by Yi-Ju Chou and Yang-Yao Niu

MS0611 - Multiphase flows with non-Newtonian materials: simulation, experiment, and machine learning

Organized by Anselmo Pereira, Rudy Valette, Elie Hachem, Manuel Alves and Alvaro Coutinho

MS0612 - Collisional Kinetic modeling in classical and plasma dynamics: numerical methods and non-linear analysis

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MS0613 - Computational fluid dynamics and heat transfer

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700 - NUMERICAL METHODS AND ALGORITHMS IN SCIENCE AND ENGINEERING

MS0701 - Numerical techniques for the simulation and model reduction of complex physical systems

Organized by Thomas Hudson and Xingjie Li

MS0702 - Isogeometric Methods

Organized by Alessandro Reali, Yuri Bazilevs, David J. Benson, RenÃ© de Borst, Thomas J.R. Hughes, Trond Kvamsdal, Giancarlo Sangalli and Clemens V. Verhoosel

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Organized by Judy Yang, Chia-Ming Fan, Pai-Chen Guan, Tsung-Hui Huang and Kuan-Chung Lin

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MS0751 - Boundary Element Method: Fundamentals and Applications

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800 - VERIFICATION AND VALIDATION, UNCERTAINTY EVALUATION AND ERROR ESTIMATION

MS0801 - DATA-DRIVEN, SURROGATE, PHYSICS-INFORMED AND GREY-BOX MODELLING FOR TREATING RANDOMNESS AND IMPRECISION IN COMPUTATIONAL ENGINEERING

Organized by Matthias Faes, Stefano Marelli, Jean-Marc Bourinet and Enrico Zio

MS0802 - COPING WITH RANDOMNESS AND IMPRECISION IN COMPUTATIONAL MECHANICS

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MS0803 - Quality of model prognosis - from lab data to structural performance

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MS0804 - Physics-Based Data-Driven Modeling and Uncertainty Quantification in Computational Materials Science and Engineering

Organized by Johann Guilleminot, Michael Shields, Lori Graham-Brady and Kirubel Teferra

MS0805 - Certification of Computer Simulations and Adaptive Modeling

Organized by Serge Prudhomme, Ludovic Chamoin, Jens Lang, Fredrick Larsson and Juan José Rédenas García

MS0806 - Verification techniques in computational physics and applied mathematics

Organized by Brian Freno and Luís Eça

MS0807 - Numerical Analysis and Design with Polymoric Uncertainties - Advanced Methods and Strategies

Organized by Michael Kaliske, Wolfgang Graf, Sigrid Leyendecker and Stefanie Reese

MS0808 - Numerical methods for verification, validation and uncertainty quantification in manufacturing, civil engineering, advanced materials and biomechanics

Organized by Naoki Takano, Kazumi Matsui, Heoung-Jae Chun, Vittorio Sansalone, Tetsuya Matsuda and Shuji Moriguchi

MS0809 - Uncertainty Quantification in Particle-Based Simulations of Fluids, Polymers, and Soft Matter

Organized by Gerald Wang

900 - STRUCTURAL MECHANICS, DYNAMICS AND ENGINEERING

MS0902 - Modelling of Structural Instability, Structural Collapse and Impact

Organized by José Santelli

MS0903 - Vehicle Scanning Method for Bridges

Organized by Yeong-bin Yang, Jong-Dar Yau, Judy P. Yang and Zhilu Wang

MS0904 - Shell and spatial structures

Organized by Francesco Marmo, Stefano Gabriele, Amedeo Manuello Bertetto and Andrea Micheletti

MS0905 - Digital twins for the design and optimisation of lightweight structures

Organized by Carol Featherston, David Kennedy, Zhangming Wu and Abhishek Kundu

MS0906 - New numerical methods for slender bodies and their interactions

Organized by Ignacio Romero, Christoph Meier, Joaquim Linn and Bastian Oesterle

MS0907 - Multiscale mechanics of soft networks: from nonwovens to polymers and living tissues.

Organized by Franck Vernerey, Nikolaos Bouklas and Catalin Picu

MS0908 - NON-MATERIAL MODELLING OF AXIALLY MOVING CONTINUA: ARBITRARY LAGRANGIAN-EULERIAN DESCRIPTION IN STRUCTURAL MECHANICS

Organized by Yury Vetyukov, Alexander Humer and Josef Kiendl

MS0909 - New Advances in Computational Modelling and Seismic Intervention Techniques of Historical Masonry Structures

Organized by Francesco Clementi, Antonio Formisano and Gabriele Milani

MS0910 - Adaptive Engineering Structures

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Organized by Thiago Ritto, Anas Batou, David Barton and David Wagg

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Organized by Eleni Chatzi, Konstantinos Agathos, Rohan Soman and Wieslaw Ostachowicz

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MS0914 - MODELING AND SIMULATION OF FUNCTIONALLY GRADED AND MULTIFUNCTIONAL MATERIALS STRUCTURES

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Organized by Chin-long Lee and Athol Carr

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Organized by Evangéline Capiez-lernout, Christian Soize, Christophe Desceliers and Marc Mignolet

MS0931 - Advances of Vehicle-Bridge Interaction Dynamics

Organized by Jong-Dar Yau

1000 - MANUFACTURING AND MATERIALS PROCESSING

MS1001 - Modeling and Simulation for Additive Manufacturing

Organized by Albert To, Yuichiro Koizumi, Andreas Lundback, Stefan Kollmannsberger, Akihiro Takezawa, Ferdinando Auricchio, Massimo Carraturo, Simone Morganti and Mamzi Afrasiabi

MS1003 - Modeling, Simulation and Optimization of Functional Materials and Advanced Manufacturing

Organized by Mahdi Bodaghi, Frederic Demoly, Giulia Scalet, Oliver Weeger and Ali Zolfagharian

MS1004 - Additive Manufacturing of Polymers - Towards the Digital Twin

Organized by Dominic Soldner, Katrin Wudy and Julia Mergheim

MS1005 - Shape Optimization for Large-Scale Problems

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MS1007 - MODELING AND SIMULATION APPROACHES OF METAL ADDITIVE MANUFACTURING ON PART-SCALE

Organized by Christoph Meier, Michele Chiumenti, Neil E. Hodge, Miguel Cervera and Wolfgang A. Wall

MS1010 - MANUFACTURING PROCESS MODELING AND THE EFFECTS OF MANUFACTURING ON THE MECHANICAL PERFORMANCE OF COMPOSITES

Organized by Patrick De Luca, Anaïs BARASINSKI, Kiyoshi UZAWA and Anthony WAAS

1100 - ATOMISTIC, NANO AND MICRO MECHANICS OF MATERIALS

MS1101 - Multiscale Modeling for Materials

Organized by YUCHIEH LO, I-Ling Chang and Chang-Wei Huang

MS1102 - Computational Nanomechanics and Nanoscale Thermal Transport

Organized by Haifei Zhan, Gang Zhang and Yuantong Gu

MS1103 - Composites, Bio-composites and Nanocomposites

Organized by Jia-Lin Tsai and Jia-Yang Juang

MS1104 - Deformation Analysis of Carbon Nanomaterial with Lattice Defects

Organized by Yi-Lun Liu, Jin-Xing Shi and Xiao-Wen Lei

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Organized by Keonwook Kang, Byeongchan Lee, Seunghwa Ryu and Akiyuki TAKAHASHI

MS1106 - Nanomechanics of defects in crystalline materials

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MS1107 - Modeling Mechanics of Materials with Voids

Organized by Matthew Lewis and Gary Gladysz

MS1108 - Topological Defects in Mechanics, Mathematics, Physics, and Beyond

Organized by Gerald Wang, Amit Acharya and Franziska Weber

MS1110 - Frontier in nano-scale graphene and AI-assisted design of graphene-like architect materials

Organized by Zhao Qin and Chi-Hua Yu

1200 - MODELING AND ANALYSIS OF REAL WORLD AND INDUSTRY APPLICATIONS

MS1201 - NON-CONVENTIONAL METHODS FOR SOLID AND FLUID MECHANICS (NMSFM)

Organized by Wojciech Sumelka, Tomasz Blaszczyk, Hongguang Sun, Jacek Leszczynski and Giuseppe Failla

MS1202 - MODELING METHODS, SIGNAL ALGORITHMS AND MACHINE LEARNING FOR EFFECTIVE NON-DESTRUCTIVE TESTING AND STRUCTURAL HEALTH MONITORING

Organized by Menglong Liu, Gongfa Chen and Fangsen Cui

MS1203 - Nonlocal models in computational mechanics: perspectives, challenges, and applications

Mirco Zaccariotto , Marta D'Elia , Ugo Galvanetto and Pablo Seleson

MS1204 - Combined finite-discrete element methods for multi-body dynamics and fracture mechanics

Organized by Ado Farsi

MS1205 - Real World Modeling and Simulation for the realization of Human-centered Society 5.0

Organized by Tohru Hirano and Seiichi Koshizuka

MS1206 - Condition assessment of railway infrastructures

Organized by Pedro Montenegro, Munemasa Tokunaga, Matsuoka Kodai and Diogo Ribeiro

MS1207 - Offshore Wind Power : Large Scale Modeling and Assesment for the Realization of Net-zero World

Organized by Takanori Uchida

MS1208 - Industrial Application of Particle Methods

Organized by Sunao Tokura, Massimo Galbiati, Brant Ross and Mamika Kawahara

MS1209 - Advanced Computing Technique and Artificial Intelligence for Realistic Social, Traffic and Economic Problems

Organized by Hideki Fujii, Eisuke Kita, Tomoaki Tatsukawa and Shinobu Yoshimura

MS1211 - Particle and Finite Element Models for Interaction, Simulation and Statistical Design

Organized by Masakazu Ichimiya, Nobuki Yamagata, Jeffrey Fong, Robert Rainsberger and Pedro Marcal

MS1213 - Modeling&Simulation of Terrestrial Flows (Terrestrial(Geosphere) hydrologic/hydraulic flow modeling&simulation)

Organized by Hiroyuki Tosaka, Makoto Nishigaki, Tomochika Tokunaga, Masaatsu Aichi and Tomonari Shiraishi

MS1214 - Advanced Modelling for Automotive Applications in CASE Era

Organized by Tohru Hirano, Kosho Kawahara, Masato Nishi and Maurizio MAGGIORE

MS1215 - Image Processing, Discretization, and Simulation of As-Built Geometries

Organized by Scott Roberts, Nagi Mansour and David Noble

MS1216 - Solid Mechanics of Elastomers

Organized by Hiro Tanaka and Hiroshi Kadowaki

MS1217 - Analysis of Real World and Industry Applications: emerging frontiers in CFD computing, machine learning and beyond

Organized by Eleni Koronaki, Anina Šarkić Glumac and Stéphane P.A. Bordas

MS1218 - Industrial Perspectives on Isogeometric Analysis and Design with Advanced Spline Techniques

Organized by Panagiotis Karakitsios and Vasiliki Tsotoulidi

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Organized by Tasnim Hassan and Katsuhiko Sasaki

MS1220 - HPC application on turbulent wind over urban model represented by individual shape of buildings

Organized by Tetsuro Tamura, Yasuaki Ito and Hidenori Kawai

1300 - INVERSE PROBLEMS, OPTIMIZATION AND DESIGN

MS1301 - Computational structural design for architecture and civil engineering

Organized by Makoto Ohsaki, Sigrid Adriaenssens, Ruy Pauletti and Yohei Yokosuka

MS1302 - Model Learning and Optimization for Nonlocal and Fractional Equations

Yue Yu , Marta D'Elia and Xingjie Li

MS1303 - ANALYSIS AND DESIGN OF STRUCTURAL DYNAMICAL SYSTEMS UNDER UNCERTAIN CONDITIONS

Organized by Hector Jensen, Jianbing Cheng, Marcos Valdebenito, Ioannis Kougioumtzoglou and Dixiong Yang

MS1304 - Optimization Method and Application

Organized by Eisuke Kita, Kazuhiro Izui, Masatoshi Shimoda, Satoshi Kitayama and Masayuki Nakamura

MS1305 - New Trends in Topology Optimization

Organized by EMILIO CARLOS NELLI SILVA, Shinji Nishiwaki, Yoon Young Kim, Glaucio Paulino, Gregoire Allaire, Daniel De Leon and Renato Picelli

MS1306 - Topological Design Optimization of Structures, Machines and Materials

Organized by Gil Ho Yoon, Akihiro Takezawa and Weisheng Zhang

MS1307 - Machine Learning and Uncertainty Quantification for Materials Design

Organized by Vahid Keshavarzzadeh, Arash Noshadravan and Johann Guilleminot

MS1308 - OPTIMIZING CIVIL STRUCTURES DESIGN - HOW TO ADDRESS MULTIMATERIAL, MULTICRITERIA AND MULTIPHYSICS PROBLEMS TO REDUCE THE GLOBAL CARBON FOOTPRINT

Organized by Fabrice Gatuingt, Guillaume Hervé-Secourgeon and Tulio Honorio de Faria

MS1309 - Recent progress in topology optimization and its applications

Organized by Junji Kato, Mathias Wallin, Niels Aage, Oded Amir, Bin Niu, Liang Xia, Mingdong Zhou and Peter Dunning

MS1311 - ADVANCED APPROACHES FOR OPTIMIZATION OF COMPOSITE STRUCTURES

Organized by Elena Raponi, Simonetta Boria, Carola Doerr, Fabian Duddeck and Dirk Lukaszewicz

MS1314 - STATISTICAL INVERSE PROBLEMS AND RELATED STOCHASTIC OPTIMIZATION METHODS FOR RANDOM HETEROGENEOUS MATERIALS

Organized by Florent Pled, Christophe Desceliers and Maarten Arnst

MS1315 - Engineering Metamaterials: Rational Design and Additive Manufacturing

Organized by Zhen Luo, Yiqiang Wang and Hao Li

1400 - SOFTWARE, HIGH PERFORMANCE COMPUTING

MS1401 - PSE (Problem Solving Enviornment)

Organized by Shinji Hioki, Masami Matsumoto and Shigeo Kawata

MS1402 - Software Design and Implementation for Next-Generation Parallel Architectures

Organized by David Littlewood, Henry Tufo, Hiroshi Okuda and Reese Jones

MS1403 - Advanced HPC Methods for Eigenvalue Problems and Beyond

Organized by Ali Hashemian, David Pardo, Victor Calo, Carla Manni and Quanling Deng

MS1404 - Progress and Challenges in Extreme Scale Computing and Data

Organized by Michael Heroux, Serge Petiton and Kengo Nakajima

MS1405 - HPC-BASED SIMULATIONS AND DATA SCIENCE FOR THE WIDE INDUSTRIAL REALM: AEROSPACE, AUTOMOTIVE, BIOMEDICAL, CONSTRUCTION, HEAVY...

Organized by Makoto Tsubokura, Mariano Vázquez, Takayuki Aoki and Andreas Lintermann

MS1406 - Portable, Efficient Implementation of Finite Elements for Mechanics Applications

Organized by Kyungjoo Kim, Mauro Perego and Nathan Roberts

1500 - FLUID-STRUCTURE INTERACTION, CONTACT AND INTERFACES

MS1501 - Computational Contact Mechanics

Organized by Peter Wriggers, Michel Raous, Giorgio Zavarise and Mike Puso

MS1502 - Fluid-Structure Interaction Algorithms and Applications

Organized by Justin Kauffman, Scott Miller and John Gilbert

MS1503 - Recent Advances in Numerical Methods for Multi-Material Shock Hydrodynamics

Organized by Ketan Mittal, Nabil Atallah, Vladimir Tomov, Guglielmo Scovazzi and Robert Rieben

MS1505 - Computational Fluid-Structure Interaction and Moving Boundaries and Interfaces

Organized by Artem Korobenko, Jinhui Yan, Ming-Chen Hsu, Kenji Takizawa, Yuri Bazilevs and Tayfun Tezduyar

MS1506 - Challenges and locks for fluid-structure interaction: from vibrations to non-linear transients in industrial framework

Organized by Vincent Faucher, Olivier Jamond, Nicolas Lelong, Benoît Prabel and Maria-Adela Puscas

MS1507 - Novel Numerical Algorithms for Fluid-Structure Interaction and Optimization for Flow Energy Converter

Organized by Ming-jyh Chern, Chao-An Lin and Tzyy-Leng Horng

MS1508 - IMMERSED BOUNDARY METHOD AND ITS NOVEL APPLICATIONS

Organized by Li Wang, Fang-Bao Tian, Wei-Xi Huang, Zhengliang Liu and Yi Zhu

MS1510 - Fluid-structure Interaction, Contact and Interfaces

Organized by Peng Du, Haibao Hu, Xiaopeng Chen, Feng Ren, Xiao Huang, Luo Xie and Jun Wen

1600 - GEOMECHANICS AND NATURAL MATERIALS

MS1602 - Computational Geomechanics

Organized by Jinhyun Choo, José Andrade, Chloé Arson, Ronaldo Borja, Richard Regueiro, WaiChing Sun and Jidong Zhao

MS1603 - Computational Methods for Snow Mechanics and Engineering

Organized by Fabrizio Barpi, Gianmarco Vallero, Monica Barbero, Mauro Borri-Brunetto and Valerio De Biagi

MS1604 - Machine learning in geomechanics and geomaterials

Organized by Jianfeng Wang

MS1605 - Validation of Numerical Modeling of Soil-Structures Interaction in Liquefiable Soils

Organized by Majid Manzari and Kyohei Ueda

MS1607 - Multiscale, Multifield, and Continuum-Discontinuum Analysis in Geomechanics

Organized by Haitao Yu, Qiushi Chen, Yiming Zhang, Xueyu Geng, Ningning Zhang, Hui Wang and Yunteng Wang

MS1608 - Particle-based numerical modeling in Geotechnical engineering

Organized by Yukio Nakata, Kenichi Soga, Mingjing Jiang and Shuji Moriguchi

MS1609 - Advanced computational modelling of wood, wood-based products, and timber structures

Organized by Josef Füssl, Markus Lukacevic, Josef Eberhardsteiner and Michael Kaliske

MS1610 - Numerical methods in geomechanics

Organized by Ryosuke Uzuoka, Kazunori Fujisawa, Toshihiro Noda and Feng Zhang

MS1611 - Computational Granular Mechanics

Organized by Hongyang Cheng, Klaus Thoeni, Xue Zhang and Vanessa Magnanimo

MS1612 - Multiscale Modeling and Numerical Stress Analysis of Prestressed Rocks

Organized by Vladimir Levin, Konstantin Zingerman and Anatoly Vershinin

MS1613 - Challenges in sea ice mechanics research - experimental investigation, theroretical description and numerical simulation

Organized by Jörg Schröder, Carina Schwarz, Doru C. Lupascu, Tim Ricken, Marcello Vichi and Sebastian Skatulla

MS1614 - Recent Advances in Computational Geomechanics

Organized by Nasser Khalili, Mohammad Vahab and Babak Shahbodagh

1700 - DATA SCIENCE, MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE

MS1701 - Applications of Artificial Intelligence and Machine-Learning Methods to Mechanics, Materials, Medicine, and Engineering

Organized by Shaofan Li, Vickie Shim, Ying Li, Harold Park and Shingo Urata

MS1702 - Machine Learning for Cardiac Modelling and Simulation

Organized by Simone Pezzuto, Francisco Sahli Costabal, Rolf Krause, Hermenegild Arevalo and Luca Dedé

MS1703 - Incorporating fundamental principles in innovative machine learning models of physics

Organized by Reese Jones, Ari Frankel, Cosmin Safta and Nathaniel Trask

MS1704 - Deep Learning in Computational Materials Science and Engineering

Organized by Shaoping Xiao

MS1705 - Data-driven and Machine learning Method for turbulence, Fluid Loads,and fluid-structure Interaction

Organized by GANG CHEN, WEIWEI ZHANG, HUI TANG and Richard P. Dwight

MS1706 - Decision-making in large-scale atomistic material simulations

Organized by Danny Perez and Thomas Swinburne

MS1707 - Uncertainty Quantification for Data-Intensive Inverse Problems and Machine Learning

Organized by Tan Bui-thanh and Andreas Mang

MS1708 - Machine Learning Based Design of Composite Materials and Structures

Organized by Seunghwa Ryu, Grace Gu, Shu-Wei Chang and Zhao Qin

MS1710 - Numerical Simulations and Machine Learning for Micro-Meteorology Predictions and Applications

Organized by Ryo Onishi, Kai Schneider, Tomoaki Watanabe, Shaoxiang Qian and Keigo Matsuda

MS1711 - Learning models for reliable predictions and decision making: methods and applications

Organized by Laura Mainini and Matteo Diez

MS1712 - Machine Learning and Computational Modeling for Mechanical Behavior of Materials

Organized by C-S David Chen, C.T. Wu and Nien-Ti Tsou

MS1713 - Deep and Machine Learning Methodology in the Context of Application to Computational Mechanics

Organized by Yasushi Nakabayashi, Yoshitaka Wada, Masao Ogino, Akio Miyoshi and Shinobu Yoshimura

MS1714 - Advances in scientific machine learning for high dimensional many-query problems

Thomas O'Leary-Roseberry , Peng Chen and Omar Ghattas

MS1715 - Intelligent design optimization of structural and mechanical systems

Organized by Jun Yan and Bin Niu

MS1716 - Data-driven approaches in computational solid mechanics

Organized by Pietro Carrara, Francisco Chinesta, Laura De Lorenzis, Siddhant Kumar, Pierre Ladeveze, Michael Ortiz and Stefanie Reese

MS1717 - Recent Advances in Scientific Machine Learning and Uncertainty Quantification Methods for Modeling Complex Systems

Organized by Ramin Bostanabad and Miguel Bessa

MS1718 - Machine Learning-Based Computational Methods in Engineering Mechanics

Organized by Alessandro Fascetti, John Brigham and Caglar Oskay

MS1719 - Advances in data-driven methods through Gaussian processes

Organized by Mengwu Guo and Anirban Chaudhuri

MS1720 - Machine-Learning Accelerated Inverse Design

Organized by Aditya Balu, Olga Wodo, Adarsh Krishnamurthy and Baskar Ganapathysubramanian

1800 - IMAGING, VISUALIZATION, VIRTUAL REALITY AND AUGMENTED REALITY

MS1802 - Computer Vision on Structural Experiments, Inspection, and Monitoring

Organized by Yuan-sen Yang

2100 - ENVIRONMENTAL, ENERGY AND RESOURCE ENGINEERING

MS2101 - Computational Mechanics for Nuclear Waste Disposal Technologies

Organized by Shin Sato, Shinya Tachibana and Stratis Vomvoris

MS2102 - COMPUTATIONAL METHODS FOR ENVIRONMENTAL FLUID FLOWS

Organized by Clint Dawson, Kazuo Kashiyama, Ethan Kubatko and Eirik Valseth

2200 - DISASTER PREVENTION AND MITIGATION, SAFETY PROBLEMS

MS2201 - Advanced Computational and Experimental Technologies for Civil Infrastructures

Organized by Sukhoon Pyo, Beomjoo Yang and H.K. Lee

MS2202 - Frontiers of Nonlinear, Impact and Instability Analysis of Solids and Structures

Organized by Daigoro Isobe, Kostas Danas, Jinkoo Kim, Sergio Turteltaub, Dai Okumura, Shingo Ozaki and Hiroyuki Yamada

MS2203 - Hyper-complex disaster simulation

Organized by Mitsuteru Asai, Antonia Larese De Tetto, Miguel Ángel Celigueta, Shunichi Koshimura and Kenjiro Terada

MS2204 - Simulation-based Disaster Prediction and Mitigation

Organized by Dongdong Wang, J.S. Chen, Sheng-Wei Chi, Pai-Chen Guan, Mike Hillman and Xiong Zhang

MS2205 - Microstructural characterization and property evaluation of materials for structural safety

Organized by Kyoungsoo Park and Tong-Seok Han

MS2206 - Advanced seismic response analysis and design

Organized by Tomoshi Miyamura, Takuzo Yamashita, Daigoro Isobe and Makoto Ohsaki

MS2208 - Physics-based Simulation of Earthquake Hazards with HPC and HQC

Organized by Takane Hori, Tsuyoshi Ichimura, Mitsuteru Asai and Thorsten Becker

2300 - INFECTIOUS DISEASES AND ENVIRONMENTAL PROBLEMS

MS2301 - Recent advances in modeling and simulating infectious disease outbreaks

Organized by Tan Bui-thanh, Leticia Ramirez and Jose Montoya-Laos

2400 - OTHERS

MS2401 - Recent advances on numerical methods and parallel solvers for the cardiac function

Organized by Luca F. Pavarino, Simone Scacchi and Christian Vergara

MS2403 - Numerical Methods for Solving Frictional Quasistatic Contact Problems

Organized by Nicolae Pop

MS2404 - Reliability of Robots

Organized by Xu Han and Shuyong Duan

MS2405 - Benchmark technologies and cases for computational acoustics

Organized by Weikang Jiang and Haijun Wu

ABSTRACTS

Designing Flexoelectric Metamaterials through Computational Strain Gradient Engineering

Irene Arias

Universitat Politecnica de Catalunya

It is well known that by deforming some materials (piezoelectrics) electricity can be produced. This functionality makes piezoelectrics ubiquitous in sensors, actuators, and energy harvesting systems. However, only a limited set of materials exhibit piezoelectricity, which limits many technologies. Applying a strain gradient to a dielectric, e.g. by bending, also generates electric fields due to the so-called flexoelectric effect, which conversely generates strains under applied electric field gradients. Unlike piezoelectricity, this effect is universal to all dielectrics, and hence of potential broad applicability. However, flexoelectric electromechanical transduction is significant only at sub-micron scales, where high strain-gradients develop, and for this reason this effect has only been characterized and is being applied in recent years. Unlike piezoelectricity, the interpretation of experiments and the design of functional devices exploiting flexoelectricity requires accurate solutions of coupled electromechanical high-order boundary value problems on complex geometries, since field gradients are required and we lack intuition on such problems.

In this talk, I will present a theoretical and computational framework to solve general flexoelectric boundary value problems based on an Immersed Boundary Hierarchical B-spline approach. I will discuss how these calculations allow us to conceive, quantify and optimize a new class of metamaterials and composites that constructively accumulate the flexoelectric effect of nonpiezoelectric micro-structural elements, and make it available as an apparent piezoelectric response at larger scales. These multi-scale metamaterials mobilize under homogeneous macroscopic strain substantial strain gradients (and polarization) in its non-piezoelectric constituents, and ensure a buildup of generated field in the material by their non-centrosymmetric arrangement. I will also discuss how large deformations can strongly enhance the flexoelectric effect in soft materials, and furthermore, how buckling-induced emergent geometric polarization can lead to tunable/switchable electromechanical materials, or to the mechanical self-assembly of large-area flexoelectric devices. Finally, I will discuss the connection between continuum theories of flexoelectricity and atomistic models based on electronic structure calculations.

Fracture and flow in porous media: A two-scale approach and spline-based discretisation

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Key Words: *Fracture, Porous media, Multiphysics, Multiscale, Fluid transport*

Since the pioneering work of Terzaghi and Biot the flow of fluids in deforming porous media has received considerable attention. However, flow in fractured or fracturing porous media, e.g. earth or rock masses, but also human tissues, has received far less attention. Yet, the presence of damage, such as cracks, faults, and shear bands, can markedly change the flow pattern and, ultimately, the physical behavior of the mixture.

Herein, we will discuss a general model for flow in progressively fracturing porous media. The two-scale approach includes flow inside stationary and propagating traction-free and cohesive cracks. The flow inside the evolving crack is assumed to be tangentially to the crack, so as to enable a two-scale approach. At the fine scale the flow in the cavity created by the (possibly cohesive) crack is modelled using a sub-grid scale model. Since the cross-sectional dimension of the cavity is small compared to its length, the flow equations can be averaged over the width of the cavity. The resulting equations provide the momentum and mass couplings to the standard equations for a porous medium, which are assumed to hold on the macroscopic scale. Examples are given not only for fluid-saturated single-phase flows, but also for unsaturated porous media, for multi-phase flows, and for non-Newtonian fluids. An assessment of the efficacy of the multiscale methodology vis-à-vis direct simulation is provided as well.

Advanced discretisation methods are needed to model a crack, which is essentially an internal free boundary. This holds a priori since higher-order continuity of the flow field is needed to ensure preservation of local mass balance, which in turn poses strict continuity requirements on the displacement field of the solid particles in view of the sup-inf condition. Isogeometric analysis seems an ideal framework to meet these requirements. We will show examples of stationary and propagating cracks and shear bands in fluid-saturated media.

Computational Mechanics-Based Digital Twin for Model Predictive Control of Autonomous UAV Landing in Adverse Conditions

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This lecture will present a two-level, data-driven, digital twin concept for the autonomous landing of aircraft in normal and adverse conditions. The concept features a digital twin instance for model predictive control; and an innovative, real-time, digital twin prototype for fluid-structure interaction and flight dynamics to inform it. The latter digital twin is based on the linearization about a pre-designed glideslope trajectory of a high-fidelity, viscous, nonlinear computational model for flight dynamics; and its projection onto a low-dimensional approximation subspace or manifold, as appropriate, to achieve real-time performance, while maintaining accuracy. Its main purpose is to predict in real-time, during flight, the state of an aircraft and the aerodynamic forces and moments acting on it. Unlike static lookup tables or regression-based surrogate models based on steady-state wind tunnel data, the real-time digital twin prototype allows the digital twin instance for model predictive control to be informed by a truly dynamic flight model, rather than a less accurate set of steady-state aerodynamic force and moment data points. The lecture will cover the fundamental aspects underlying the construction of the two-level digital twin concept and its verification by numerical simulation. Most importantly, it will also report on its preliminary flight validation in autonomous mode for an off-the-shelf unmanned aerial vehicle instrumented at Stanford University by Marco Pavone and Joe Lorenzetti.

From Engineered Metastructures to Natural Seismic Metamaterials: Theory, Computational Aspects and Experiments

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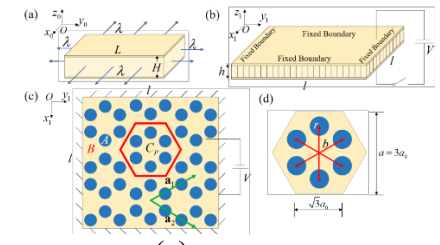
Key Words: *acoustic metamaterial, bandgap, forestation, Rayleigh wave, seismic metamaterial*

The recent surge in the number of studies on seismic metamaterials is testimony to the fact that the concept of photonic crystals, phononic crystals and acoustic metamaterials [1-3] is no longer limited to basic theories and dynamic characteristics. Apart from the peculiar observation including negative stiffness, negative mass density negative refraction properties, etc., auxetic metamaterials that govern negative Poisson's ratio, nonreciprocal wave phenomena, origami/kirigami effects also find potential applications in geophysics and earthquake engineering [4-5]. Except man-made synthetic resonators/metastructures, recently forest trees at geophysical scale are reported as naturally available seismic metamaterials with capability to mitigate ground born ambient vibrations and incoming seismic waves at subwavelength frequency region. The work to be presented here elaborates a class of materials and structures ranging from engineered phononic crystals and acoustic metamaterials in Fig (a,b) to natural seismic metamaterials in Fig. (c,d) that show exotic yet with outstanding application potentials. Besides discussing the peculiar yet wonderful wave propagation characteristics of periodic structures for wave active control, topological protected interface modes, etc., the exciting wave dispersion response that found applications for manipulation Rayleigh wave and possible forestation as a means for geographical regional isolation against ground surface wave motion will also be presented.



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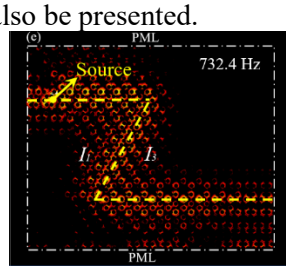

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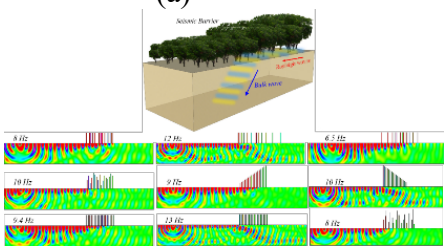

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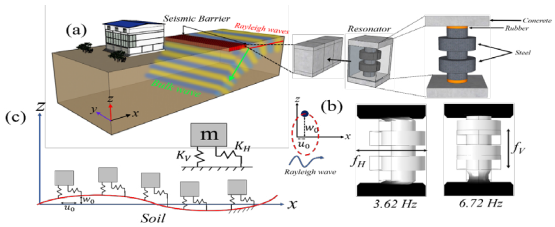

(d)

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Development of New Rocket Propulsion System "Rotating Detonation Engine"

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Key Words: *Detonation, Rotating Detonation Engine, CFD, Chemical Reaction*

Detonation wave, you may not be familiar with. It is a combustion wave propagating at supersonic speeds, and so there is a preceding shock wave in front of the exothermic reaction zone. In recent decades, detonation has attracted attention for use of a new type of aerospace propulsion engine so called “detonation engine”, since the detonation engine has higher theoretical thermal efficiency than the conventional rocket engine. Our research group, in collaboration with Nagoya University, has successfully demonstrated the world’s first space flight of detonation engines on July 27, 2021 [1].

We are working numerically to elucidate the fundamentals for detonation combustion and to predict the performance of the designed combustor geometry of “Rotating Detonation Engine (RDE)”, which is one of detonation engines, by solving the compressible flow with chemical reactions.

For RDE, there are some problems to be solved such as continuity and heat load. Here, we focus on two topics. On is the ozone addition to the hydrogen oxygen premixed gas to improve its characteristics for detonation engine, and the other is the investigation of newly designed combustors, such as side wall injections and diverging combustor geometry [2].

The ozone sensitization due to the O radical produced via ozone thermal decomposition is attracting attention as a mean of improving the detonation stability and extending its limits. Our numerical results show that the ozone can be expected to help to the complete the combustion faster and improve the thermal efficiency.

A series of numerical simulations predict the thrust performance by changing the geometrical parameters of length and shape of RDE combustor and the injector configuration, and the simulation results indicate the appropriate design of RDE. RDE is the new type of aerospace propulsion engine, and its optimal combustor shape and configuration is not clarified yet. Therefore, based on our numerical results, we will propose new combustor geometry to improve the stability and performance.

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Computational Hemodynamics for Clinical Applications – Crossroad between Patient-Specific Simulation and Machine-Learning Techniques –

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Key Words: *Patient-Specific Simulation, Cerebral Circulation, Revascularization, Multimodal Medical Image, Machine Learning*

Cardiovascular disease such as heart disease or stroke is one of main causes of death in the world. A patient-specific simulation has been widely used not only for scientific study to elucidate mechanism between hemodynamics and cardiovascular diseases but also for clinical applications to predict blood flow after surgery. Since carotid artery stenosis is a major risk factor for a stroke, patients with severe carotid artery stenosis often undergo revascularization surgery such as carotid artery stenting to prevent a future stroke. Predicting the blood flow in the brain after the surgery is very important to determine the most suitable surgery for the patients,

The surgery affects the blood flow in the brain as well as in the entire circulatory system. In order to reflect the patient's conditions in the multi-scale cardiovascular simulation, geometric and physiological parameters derived from clinical data are applied to the region of interest with the literature data for the rest of circulatory system[1]. Thus, quantifying the impact of uncertainties in the data on simulated quantities is an essential task to obtain reliable results. However, uncertainty quantification is time-consuming and computationally expensive for routine clinical diagnosis. The authors have been developing a data-driven surrogate model using machine learning technique and applied the model for risk assessment of a cerebral hyperperfusion condition, which is one of complications after revascularization of stenosis in the carotid artery[3]. In the plenary lecture, the recent advances in the multi-scale cardiovascular simulation will be presented as well as a future perspective of machine learning in the patient-specific simulation for clinical applications.

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Deep Materials Modeling and Design

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Key Words: *Materials Modeling, Materials Design, Deep Learning, Composite, Metals, Bioinspired Materials*

Materials modeling and design play a central role in mechanical applications. In this talk, I will present our three ongoing efforts using deep learning techniques to advance our materials modeling and design capability. The first is on generalizing a deep material network (DMN) to capture microstructural features using a graph neural network (GNN). We link microstructural features of RVEs to microstructural descriptors of DMN by introducing GNN into DMN architecture. A microstructure's topologies and features are utilized as input data for GNN. Through a series of message passing processes of GNN from the input, the extracted embedding vector from the microstructure can be used to find the correlations between microstructural descriptors of DMN, which correspond to different RVEs, through an end-to-end offline training process of GNN-DMN network architecture. Once the network is trained, it can be viewed as a unified composite material modeling for RVEs with similar morphologies and be utilized for online predictions of material nonlinear behaviors due to the inherent merits of DMN. The effectiveness and efficacy are demonstrated for two-dimensional two-phase composite materials with different morphologies, including matrix-inclusion, amorphous and anisotropic geometries. The second part of my talk is on developing a surrogate model for crystal plasticity using GNN and recurrent neural network (RNN). To enhance the accuracy of spatial-temporal prediction, we introduce an independent self-weight for message passing in the GNN layer to distinguish the message from the grain itself and those from the neighboring grains. Strain incompatibility is integrated into the loss function as a physics-informed regularization term. The proposed deep learning model is trained on the dataset generated by a high-fidelity crystal plasticity simulation to predict the stress-strain response and microstructural evolution under complex loading paths. The accuracy of the surrogate model on spatial-temporal prediction is shown to be significantly improved. We also demonstrate the generalizability of the proposed surrogate model on various polycrystalline geometries. The third part of my talk is on designing bioinspired microstructures with target properties. Distinct from engineering materials, biological structural materials are often composites of hard/brittle minerals and soft/ductile proteins arranged into complex microstructures with remarkable mechanical properties. A property-prediction model for bioinspired microstructures using supervised learning and a framework for designing bioinspired structural materials with tailored mechanical properties using reinforcement learning will be addressed.

Empowering data-informed engineering from smarter data, sensing and hybrid modelling

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Key Words: *Model Order Reduction, Active Learning, Data-Driven modelling, Twins*

Data has not an intrinsic nature, data exist with respect to a specific mission, the one of performing diagnosis, or the one of enabling the construction of a model able to make efficient (fast and accurate) prognosis, and the subsequent prescriptive actions and decisions.

In engineering data is expensive in what concerns its collection, transmission, storage and analytics. For this reason, collecting the right data, at the right place and instant is preferred. Active learning constitutes a timely research topic, and more importantly, physics-aware active learning can profit of the existing knowledge, in conjunction with the previous collected data, for driven the data acquisition.

With the data available, machine learning can proceed for extracting a model relating the input-data with the output-data. However, when the amount of data is small, frugal AI and frugal machine learning techniques must be considered. For reducing the data needs, physics informed (from the physics-based model or from the thermodynamical consistency), data-augmentation, data reduction (auto-encoders), reinforced learning, transfer learning (augmented learning), … allow defining efficient (fast and accurate) learning technologies.

Now; that models are available, engineering can profit: Data-assimilation, monitoring, diagnosis, prognosis, prescriptive control and decision making, can operate, in a supervised or unsupervised manner, profiting of the advanced visualization technologies: virtual, augmented and hybrid reality, for creating a physics-aware digital twin, also called Hybrid Twin for emphasizing the two coexisting modelling frameworks: the physics-based (operating in real-time thanks to the use of advanced model order reduction techniques, as for example the so-called PGD) and the data-driven models (as just indicated physics informed).

Machine-Learning based Computational mechanics as a powerful tool for engineering and science

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Key Words: *Physics-Informed Neural Network, Machine Learning, Computational mechanics*

Nowadays, the Physics-Informed Neural Network (PINN)-based computational solid mechanics is being rapidly developed, although it is currently still in its infant stage. It has been becoming a game-changer for computer modelling and simulation for engineering and science.

Firstly, this talk will review the most recent developments of PIINN for mechanics, including solid mechanics, fracture machines and fluid mechanics. The main challenges in application of PINN to computational mechanics are discussed.

Second, in PINN, the loss function plays a critical role. It is still an opening question for developing an effective, robust, and general loss function for solid mechanics problems, although a couple of approaches, for example, the energy-based loss function and the collocation loss function, have been proposed to create the loss function. We proposed a new way to formulate the loss function based on the Least Squares Weighted Residual (LSWR) method for PINN-based computational solid mechanics. Using the LSWR method, the proposed loss function is tailored to a dimensionless form, and only one parameter is required to be determined based on the spacing of the sample points. It has been proved that the proposed LSWR loss function is effective, robust and accurate for both the displacement and stress fields. Meanwhile, the effectiveness of the proposed LSWR loss function can be easily extended to for geometric nonlinearity problems with transfer learning. The proposed LSWR loss function provides an effective way for PINN based computational solid mechanics and is straightforward to be implemented

Third, the recent research in the speaker's group on PINN will also be reported in this talk. It has proven that physics-informed machine learning will be the new generation of a computer modelling framework for mechanics.

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Discrete Crack Models in Regularized Fracture Mechanics for Mesh-based and Mesh-free Methods

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Key Words: *Representative Crack Element (RCE), Phase-field Fracture, Eigenfracture*

The explicit representation of cracks in discretised models via domain bounds, the mesh, or special ansatz functions is the most direct way to model fracture and common use in computational mechanics with field discontinuities. In addition, pure continuous models are frequently applied to the simulation of weak and strong discontinuities, for instance nonlocal plasticity and nonlocal damage formulations. The latter models gain more flexibility for the numerical discretisation and introduce a length-scale parameter for the description of the fracture process or localisation zone.

Investigations on the energetical balance during fracture dates back to the contributions of GRIFFITH and IRWIN, and has yielded later a fully variational formulation, the *free-discontinuity problem* [1], where the displacement field as well as the location of displacement discontinuities are unknown a priori. Regularised formulations of the free-discontinuity problem like the *phase-field method for fracture* [2] and the *eigenfracture* approach [3] have gained much attraction because they combine precision of discrete and flexibility of continuous approaches to fracture mechanics.

In the focus of this talk is the additive decomposition of the spatial derivative of the displacement field in the presence of a crack into an absolutely continuous part and a jump part, which is shown via the space of special functions of bounded variations [1]. The former part describes the deformation of the bulk material at the crack surface, whereas the latter part focuses the contribution of crack opening. However, continuous fracture models calculate the overall derivative of the displacement field and do not provide this decomposition, which is necessary for a precise description of the bulk material and processes inside the crack gap. In order to overcome approximatively decompositions via artificial split models, the framework of *Representative Crack Elements* is developed, solving the decomposition as a variational problem.

Illustrative applications to elastic and inelastic bulk materials, to crack surface friction and finite deformations, as well as to multi-physical problems are used to compare to experimental observations and numerical results from discrete fracture models. Simulations are performed by means of the phase-field approach and the eigenfracture method using the mesh-based *Finite Element Method* and the mesh-free *Material Point Method*.

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Opportunities for Machine Learning in Computational Mechanics

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Key Words: *Neural Networks, Bayesian Inference, Bayesian Physics-Informed Neural Networks*

Understanding real-world dynamical phenomena remains a challenging task. Across various scientific disciplines, machine learning has advanced as the go-to technology to analyze nonlinear dynamical systems, identify patterns in big data, and make decisions around them[1]. Here we systematically compare two families of machine learning tools and illustrate their applications in computational mechanics: neural networks and Bayesian inference[2].

Neural networks minimize a loss function to optimize the network parameters, without any prior knowledge of the underlying physics. Physics informed neural networks expand the loss function by an additional physics term and also optimize for physics parameters. In addition to plain neural networks, physics informed neural networks not only interpolate the training data well, but also extrapolate and predict future behavior. We illustrate the features of physics informed neural networks for several biomedical applications[3].

Bayesian inference maximizes a prior-weighted likelihood function to estimate posterior distributions of model parameters. It can be combined with plain neural networks or physics informed neural networks to ignore or integrate the underlying physics. Bayesian inference not only infers model parameters to fit the training data, but also provides credible intervals to quantify the quality of the model. We illustrate the potential of Bayesian inference for dynamical systems in the life sciences[4].

We conclude by discussing the inherent advantages and disadvantages of neural networks, Bayesian inference, and a combination of both to provide guidelines which approach to select. We anticipate that our study generalizes to a wide variety of nonlinear dynamical systems and opens new opportunities for machine learning in computational mechanics.

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On law- and data-based methods

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Key Words: *Finite Element Method, Smoothed Finite Element Method, Machine Learning, Artificial Intelligence, numerical methods, computational methods*

Machine learning methods [1], such as the Artificial Neural Networks (ANNs), have been applied to solve various science and engineering problems. TrumpetNets and TubeNets were recently proposed by the author [2][3] for creating two-way deepnets using the standard finite element method (FEM) [4] and S-FEM [5][6]as trainers. The significance of these specially configured ANNs is that the solutions to inverse problems have been, for the first time, analytically derived in explicit formulae. Such advancements have shown that fundamental understanding on physics law-based and data-based methods has found critical for development of novel methods for various types of engineering problems [9][10][12].

This paper discusses general issues related to law-based [4]-[8] and data-based [1][3] methods, including the principle, procedure, predictability, and property of these two types of methods in dealing with different types of problems. We present also a novel neural element method (NEM) [9][10] as a typical example of a possible combination of these two types of methods. The key idea in NEM is to use artificial neurons to form elemental units called neural-pulse-units (NPUs), using which shape functions can then be constructed, and used in the standard weak and weakened-weak (W2) formulations to establish discrete stiffness matrices, similar to the standard FEM. Detailed theory, formulation and codes in Python and numerical examples are presented to demonstrate this NEM. For the first time, we have made a clear connection, (in theory, formulation, and coding), between ANN methods and physical-law-based computational methods. We believe that his novel NEM changes fundamentally the way approaching mechanics problems, and opens a possible new window of opportunity for a range of applications. It offers a new direction of research on un-conventional computational methods. It may also have an impact on how the well-established weak and W2 formulations can be introduced to machining learning processes, for example, creating well-behaved loss functions with preferable convexity.

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A semi-resolved CFD-DEM approach for particulate flows with thermal convection

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Key Words: *Particulate flows, CFD-DEM, Semi-resolved CFD-DEM, Thermal convection*

Particulate flow has a wide range of industrial applications and is frequently modeled with coupled CFD-DEM approaches. In this work, we first identified a simulation gap between the resolved CFD-DEM and unresolved CFD-DEM through a size effect study. We then analyzed the error sources of the conventional unresolved CFD-DEM when modeling particulate flows with comparable mesh size and particle diameter. We finally developed a semi-resolved CFD-DEM model[1, 2], which combines the advantages of both resolved and unresolved CFD-DEM models. The semi-resolved CFD-DEM uses a drag force model to characterize particle-fluid interaction, while the relative velocity in the drag force model is corrected through kernel-based approximations on the neighboring fluid cells rather than simply taking values in the local cell containing the concerned particle, and the void fraction in the force model is corrected as well. A number of numerical simulations including the sedimentation of single particle, separation of particles in a fluidized bed, spouted bed with heat particles, particulate flows in complex porous media, additive manufacturing (selective laser melting and direct laser deposition) have been conducted. Numerical results from different CFD-DEM approaches are compared together with experimental data. It is shown that the presented semi-resolved CFD-DEM bridges the simulation gap between the resolved CFD-DEM and unresolved CFD-DEM while it is as efficient as the conventional unresolved CFD-DEM and as accurate as the resolved CFD-DEM.

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Hierarchical Deep Learning Neural Network (HiDeNN)-FEM- AI for process design and performance prediction of material systems

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We propose a mechanistic Artificial Intelligence (AI) framework, called Hierarchical Deep Learning Neural Networks or HiDeNN-AI [1,2,7,8] for discovering the multiscale linkage of process-structure-property of additive manufacturing systems. The HiDeNN-AI discovery has three sequentially executed steps: (1) using available data to characterize an unknown physical process in manufacturing, (2) enriching the database and training with mechanistic knowledge coming from the system identification in step (1) with uncertain parameters to create a reduced order model with uncertainty, and (3) using the reduced order model to generate sufficient data to discover new robust mathematical principles that are able to (a) perform predictive solutions for design and optimization, and (b) provide simple relationship for online monitoring and control. We have applied this HiDeNN-AI framework to address the Air Force Research Lab (AFRL) AM modeling challenges [3, 4, 5]; and for the prediction of the as-built mechanical properties [6]. To further enhance HiDeNN-AI, a reduced-order modeling method accounting input uncertainty, called the Tensor Decomposition (TD) [7], is being developed. The so-called HiDeNN-AI-TD is expected to solve the general engineering design and manufacturing problems in high dimensional space-time-parametric domains at deep discount in computational cost. Once the offline database is set up, the mechanistic machine learning module of HiDeNN-AI can be activated for process design, real time system monitoring and control or the identification of key processing parameters for the desired performance of the manufactured material systems with uncertainty quantification. Various results comparing the HiDeNN-AI-TD approach with the conventional machine learning models will be shown using real-time IR in-situ measurement, and high-frequency thermal signatures for the predictions of mechanical properties and the detection of lack of fusion and keyhole porosities. Similar applications to polymer matrix composites will be presented.

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Recent Advances of Constitutive Models of Soft Smart Materials - From Molecular, Network Scales to Continuum Scale

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Key Words: *Constitutive model, Hydrogel, Molecular Dynamics, fracture of hydrogels*

Hydrogel is a type of synthetic polymers composed of cross-linked polymer network and water. A polymer network can imbibe copious amounts of water and swell, which can be used in many potential applications, such as stretchable conductors, tissue engineering and fire resistance materials. Before these applications, hydrogels should be studied carefully. We have studied the mechanical and thermal properties of hydrogels from the molecular scale to the continuum scale. In this presentation, the multi-scale study of hydrogels will be discussed. Such as the ab-initio simulations are carried out to investigate the force field parameters of hydrogel and the randomly crosslinked molecular structure of hydrogel is built by simulating the reaction process of monomer and crosslinker. The diffusion property of solvent molecules and heat conduction in hydrogels with different water contents are simulated by using Molecular Dynamics method. Besides, the swelling, mechanical, as well as the phase transition behaviours of environmental sensitive hydrogels (such as pH sensitive, thermal sensitive and photosensitive) are investigated by continuum theory and FEM approach. As current constitutive theories face challenges when predicting the extremely large deformation and fracture of hydrogels, and in order to reveal the fundamental mechanism of the various mechanical behaviours of hydrogels from bottom up, we also proposed a proper hydrogel network model to provide a better approach to bridge the gap between the micro-structure and the macroscopic mechanical responses. This presentation will summarizes the theoretical and numerical researches on the different hydrogel models, aiming to provide new insights into the effect of microstructure on the swelling-deswelling process, hyperelasticity, viscoelasticity and fracture of hydrogels. In order to verify the proposed constitutive models, we have carried out some experimental studies. Furthermore, some interesting experimental results will be presented in this talk also.

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Wings at low Reynolds numbers and lifting line theory

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Key Words: *Mode C instability, Hairpins, Laminar separation bubble, Wing-tip vortex, Cellular shedding, Streamwise vortices*

Low Reynolds number flows past UAVs, MAVs and drones have gained significant interest because of their surveillance, communication, weather monitoring, etc. We first study the transition of flow past an end-to-end wing [1]. The flow becomes unsteady beyond Re=600 approximately via the primary instability of the wake leading to vortex shedding. Three-dimensionality sets in at Re~1280.9 via mode C instability and hairpin vortices. The spatio-temporal structure of the flow is examined via spanwise variation of lift coefficient. Interaction of the shear layer vortices with the separated boundary layer leads to formation of a Laminar Separation Bubble (LSB) at Re~20,000, causing a delay in flow separation. The airfoil experiences a very significant increase in lift and decrease in drag. The primary mechanism of formation of LSB is found to be two-dimensional. Unlike the frequency of vortex shedding, the frequency of shear layer vortices experiences a sharp change at the onset of LSB.

The main objective of the work is to study the effect of wing-tip vortices on the transition of flow on a finite wing and its aerodynamics at low Reynolds numbers. Numerical simulations for flow past a finite rectangular wing with NACA 0012 section at Re=1000 for various semi-aspect ratios ($0.25 \le sAR \le 7.5$) over a range of angle of attack ($0° \le \alpha \le 14°$) reveal streamwise vortices, which increase in strength and number to occupy an increasing spanwise extent with increase in α. Unlike the prediction from the Lifting Line Theory (LLT) by Prandtl [2], they result in non-monotonic spanwise variation of local force coefficients for $\alpha > 8°$. Viscous and pressure drag dominate for low- and high-sAR respectively. The time-averaged drag coefficient first decreases and then increases with increase in sAR. This is in contrast to the prediction from LLT and will be discussed in detail in the presentation. Vortex shedding, for $\alpha = 14°$, is single cell and parallel for $sAR < 3$. Shedding is in two cells with oblique angle that varies with time, leading to large spanwise variation in rms of local force coefficients for higher sAR. Various type of dislocations, reported earlier in wakes of bluff bodies [3], are seen for different α and sAR. Dislocations, for $\alpha = 14°$, appear at same spanwise location for sAR=3 and at different spanwise locations for $sAR \ge 4$. Vortex shedding for $\alpha = 14°$ and sAR=5 exhibits one cell structure in the near- and two-cell in the far-wake due to splitting and reconnection of vortices near midspan in the moderate wake. Linkages form between counter rotating spanwise vortices for $sAR \ge 1$. Additional linkages between shed- and wing-tip vortices are observed for lower sAR. The strength of wing-tip vortex increases with α. At each α, the strength and radius of its core, estimated using a forced-free vortex model, increases up to a certain sAR beyond which it is approximately constant. The incompressible flow equations are solved via a stabilized finite element method [4].

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Isogeometric Analysis: Some recent advances and applications

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Key Words: *Isogeometric Analysis, Coupled Problems, Phase-field Modeling*

Isogeometric Analysis (IGA) is a successful simulation framework originally proposed by T.J.R. Hughes et al., in 2005, with the aim of bridging Computational Mechanics and Computer Aided Design. In addition to this, thanks to the high-regularity properties of its basis functions, IGA has shown a better accuracy per degree-of-freedom and an enhanced robustness with respect to standard finite elements in many applications - ranging from solids and structures to fluids, as well as to different kinds of coupled problems - opening also the door for the approximation in primal form of higher-order partial differential equations.
After a concise introduction of the basic isogeometric concepts, this lecture aims at presenting an overview of some recent advances in IGA with a special focus on coupled problems where the characteristics of IGA seem to be of great advantage. In particular, applications that will be discussed include the simulation of fluid-structure interaction in different contexts like, e.g., biomechanical problems, studies on the effect of mechanically-induced stresses on prostate cancer growth, thermo-mechanical simulations of additive manufacturing processes, electro-mechanical simulations for biological tissues, and the use of phase-field modeling for fracture and topology optimization problems or for predicting the polarization evolution in elastic ferroelectric materials. The last part of the presentation will be finally devoted to the description of a simple, accurate, and inexpensive simulation technique for laminated structures, allowed by the peculiar IGA features.

Parametric Model Order Reduction for Fluid and Solid Objects

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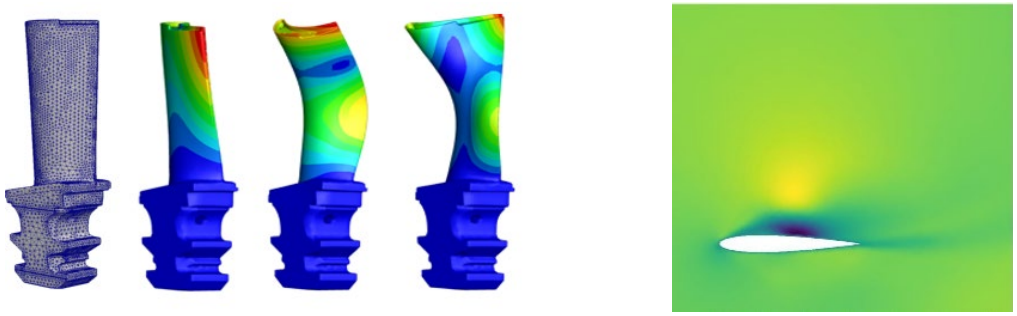
Key Words: *Model order reduction, Multiphysics Problems, Large-size computational anaysis, Computational structural dynamics, Computational fluid dynamics*

The large-size computation conducted in the engineering field is complex, higher-dimensional, and occasionally highly nonlinear. While a variety of the direct numerical analysis have been attempted for the solid, fluid and thermal analysis, its computational burden still remains excessive. In order to reduce such computational load, approaches such as parallel computing and model order reduction have been attempted. Whilst the parallel computing may reduce the computational time significantly as the computation is performed in a distributed manner, it will not reduce memory requirements.

Instead, the model order reduction (MOR) will be considered. MOR aims to reduce the dimension of the higher-dimensional full order representation to a smaller one along with the minimal discrepancy. It will be efficient in terms of both computational speed and memory requirement. Approaches for MOR can be widely categorized into the following two categories: intrusive and non-intrusive MOR. The intrusive MOR is dependent on the governing equation while the non-intrusive MOR does not require knowledge of the governing equation. In this paper, an overview of the model order reduction and numerical results will be presented. The examples include intrusive MOR for the solid analysis [1] and non-intrusive MOR for the fluid analysis [2]. By examining such examples, efficiency and accuracy by various MOR approaches will be demonstrated.



(a) Intrusive MOR for the solid analysis[1] (b) Non-intrusive MOR for the fluid analysis[2]

Fig. 1. Numerical results by the intrusive and non-intrusive model order reduction

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A Topology Optimization approach towards fluid flow design problems

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Key Words: *Topology optimization, Fluid flow design problems*

Topology optimization (TO) is a computational engineering tool used to provide optimized geometries, with highly attractive applications in the areas of structural and fluid flow path designs. The main goal of TO is to solve a material distribution problem within a design domain considering an objective function and a set of possible constraints. In the case of fluids, the design variable values {1} and {0} usually indicate the regions of the domain where the fluid is free to flow (*fluid*) or is restricted to flow (*solid*), respectively. The use of TO for fluid problems began with laminar flows, and the current most challenging applications of TO methods for fluid flow design include the consideration of turbulent and compressibility effects. Another important aspect is the design of blood flow devices, since blood is a living fluid, subject to blood damage (hemolysis and thrombosis). Thus, this lecture will present the main aspects of TO for fluid flow design covering laminar and turbulent flows, Newtonian and non-Newtonian fluids, blood damage (hemolysis and thrombosis), and incompressible and compressible flows. The TO formulation will be presented based on the continuous design variable formulation, and also on a recent development based on discrete design variables and sequential integer linear programming. Examples include the design of fluid flow channels/devices, and flow machine rotor/volute topologies.

Prediction of fatigue crack propagation using effective regularization techniques for regression problems

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Key Words: *Fracture Mechanics, Machine Learning, Surrogate Model, Imbalanced Frequency Problem*

This study presents the capability and applicability for fatigue crack propagation evaluation using the latest machine learning. Fatigue crack propagation includes several governing laws and computation methods which are elastic stress field, stress intensity factors, Paris' law and criterion of crack propagation direction. Crack propagation phenomenon simultaneously occurs with these laws. The computation time is needed for one case of crack propagation. Many crack propagation paths for a training are computed as training data in 2-dimension using s-version finite element method, however a machine learning can easily predicted interpolated crack propagation path and its rate very shortly than a finite element analysis.

Three training levels are examined. In 1st training level, crack position vector, propagation direction vector and stress intensity factors are for input parameters. In 2nd training level, crack position vector, crack propagation direction vector, six stress components around crack tip are for input parameters. In last training level, only crack position vector and crack propagation direction vector are trained as input parameters. The last level requires only geometrical configuration to predict crack propagation. In order to simplify the problem, all of parameters are completely determined as constant values. The simulation can represent curved crack path by incremental crack propagation computations. As a result of comparisons between each level, the 1st level exhibits the highest reproducibility. If the same computation results as the 1st level, the last level requires 10 times training data and time to get convergence of the convolutional neural network system. The accuracy of all phases presents the common deviation from the correct solution. The deviation appears at the beginning of crack growth involving steep crack direction change. As a result, data augmentation is employed for the first several computation steps on each initial crack angle, and training data of cracks with fine intervals.

Interaction of two cracks propagation is predicted and evaluated so that we'd like to enhance the prediction ability of crack propagation. When two cracks are very closed and interaction occurs evidently, data augmentation also should be employed because of very close cases less than usual state as concerns with distance of two cracks. The dense distribution of the training data and the augmentation produce highly accurate prediction of crack propagation in case of very close cracks. A quality of training data largely affects an ability of a prediction. The important thing is that the training data should contain data to predict some phenomena. We'd like to discuss the results of several learning examples and show the applicability of the machine learning to the actual engineering problem with high accuracy.

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Virtual elements in engineering sciences

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Key Words: *Virtual elements, fracture mechanics, contact mechanics, homogenization, Kirchhoff plates*

Virtual elements (VEM) were developed during the last decade and applied to various problems in solid mechanics. The method includes elements that can have arbitrary shape including non convex polyhedra. This flexibility with respect to the geometry can be explored and utilized within engineering applications for specific problems.

This lecture will cover several applications of the virtual element method in the area of solids mechanics which are related to

- contact and interfaces,
- fracture using classical and phase field approaches,
- homogenization of polycrystal microstructural response,
- design C1-continuous ansatz spaces for plates and gradient elasticity

For these problem classes we will discuss the pros and cons of virtual elements for efficient, reliable and robust solutions in the engineering world.

A Multiscale Computational Framework for the Simulation of Graphene Nanoplatelets

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Key Words: *Graphene Nanoplatelets, Multiscale, Homogenization, Random Fields*

In this paper, a multiscale computational framework is developed for the simulation of graphene nano-platelets (GnPs) used as reinforcements in composite materials. GnPs, which consist of multiple graphene sheets connected by van der Waals forces, are modelled following the Molecular Structural Mechanics (MSM) approach [1] using energy equivalent beam and spring elements. Stone-Wales as well as single and double vacancy defects are considered in the graphene sheets [2]. The apparent mechanical properties of GnPs are described by random fields, obtained by means of computational homogenization [3]. Parametric investigations are carried out to examine the effect of the number of constituent graphene layers, as well as of defect type and density, on the mechanical properties of GnPs.

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Experimental and Theoretical Research on the Cyclic Deformation of NiTi Alloys after Hydrogen Charging

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Key Words: *NiTi shape memory alloy, hydrogen diffusion, scale conversion*

NiTi shape memory alloys inevitably come into contact with hydrogen under certain service environment, which has influence on its mechanical behavior. In this work, the effect of hydrogen on the cyclic deformation of NiTi alloys is revealed experimentally and theoretically through cyclic tensile-unloading experiments of super-elastic NiTi alloy wires after hydrogen charging.

In the first cycle of the strain-stress curves, the transformation platform of loading curve is divided into two parts after ex-situ hydrogen charging of NiTi alloy wires. With the presence of hydrogen, initial stress of second transformation (the second stage of transformation platform) and the reverse transformation increases, and transformation platform is shortened. The longer the charging part is, the earlier the second transformation starts. In addition, hydrogen charging time and charging length (the length of hydrogen charging part) increase residual strain during loading ang unloading process. The reason is that hydrogen hinders transformation of NiTi alloys.

As the number of loading cycles increases, the segmentation of transformation platform “disappears”. Subsequently, this phenomenon reappears. The transformation starting stress of charging specimens decreases more rapidly than that of the as-received. Hydrogen has a promoting effect on the generation of internal stresses in NiTi alloys. And the hindering effect of hydrogen on transformation and the promoting effect on internal stress are competing mechanisms.

The aim of this paper is to establish a mechanical-diffusion coupled constitutive model of NiTi shape memory alloys, which regards the above effects of hydrogen on mechanical behavior of NiTi alloys. In order to calculate the hydrogen concentration, stress and strain fields of NiTi alloy wires, and obtain the overall thermomechanical response of NiTi wire.

At the same time, in order to reduce the computational cost faced by the software when calculating the fully coupled analysis, the diffusion theory and scale conversion rule are introduced, combined with the developed constitutive model to describe the macroscopic thermomechanical response of NiTi alloy wires. The prediction results of the two methods are in good agreement with the experimental data.

Harmful Microstructures in Fatigue: Influence of Grain Morphologies and Orientations on Local Stress Distributions

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Key Words: *Cellular Automaton, Micromechanics, High Cycle Fatigue, Grain Shape Effect*

Predicting where and especially when fatigue cracks will occur is a complex mater. In addition to the crystallographic orientation of the grain itself, the configuration of its neighborhood has a strong influence on the strain and stress levels generated during fatigue solicitations. As it is the worst configurations out of a large number of grains and neighborhoods that will drive the fatigue performance of a material, extreme value statistics have to be used. To do so, large set of data have to be generated in a reasonable CPU time.

Mean-Field Homogenization methods are fast, but they do not provide enough statistical information to be relevant. Although Full-field Finite Element simulations does provide a precise quantification of the neighborhood effect, the associated CPU times are very high and gathering sufficient data for extreme data statistics will require very high CPU times. There is a sort of compromise between these two approaches in the method based on Cellular Automaton (AC). Its CPU time is several orders of magnitude lower than Finite Element simulations and still provides precise localisation information. Thus, it is a relevant tool for gathering enough data to describe the statistical nature of the neighbourhood effects in polycrystals.

In the present paper, the AC method is applied to a microstructure with complex grain shapes. As an extension to Bretin et al. on close-to-equiaxal microstructure [1], the Eshelby Equivalent Inclusion Method (EIM) [2, 3] was developed for grains with various revolution ellipsoid shapes. The local stress field for different microstructures configurations were calculated. A large variety of aspect ratios and relative spatial orientations were documented for a 316L stainless steel, material known for its strong anisotropic elastic properties. The results were analysed to identify best as well as worst configurations for fatigue performance.

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Mechanical Stimuli in Prediction of Trabecular Bone Adaptation; Numerical Comparison

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Key Words: *Trabecular Bone, Bone Adaptation, HR-pQCT*

Adaptation is the process by which bone responses to changes in loading environment and modulates its properties and organization to meet the mechanical demands. Trabecular bone, the spongy component of many bones, undergoes significant adaptation when subjected to external forces. It was found that intensive mechanical stimulation results in thicker and mechanically stronger bones and bone morphology with individual elements of this bone tissue, *trabeculae*, aligned along the loading direction [1]. In contrast, a lack of mechanostimulation induces a bone-mass reduction, thinning of trabeculae, and deterioration of mechanical properties [2]. Load-induced adaptation is implemented through resorption of old and fractured bone and formation of a new bone material. These processes are hypothesized to be driven by mechanical stimuli of bone-matrix deformation sensed by bone mechanosensory cells [3]. The exact nature of mechanical stimuli triggering bone resorption and formation activities in response to external loads is currently unknown.

This study aims to compare different mechanical stimuli on their ability to trigger load-induced adaptation in trabecular bone. To achieve this, developed 3D unit cells of trabecular lattice are developed with bone marrow in its intertrabecular space, reconstructed from two sets of high-resolution peripheral computed tomography (HR-pQCT) scans. The first set includes baseline scans of distal tibia of a human participant, the second one comprised scans of the same participant after a six-months-long high-impact exercise. The finite-element method is implemented for the baseline model loaded in compression, tension, and shear to calculate the magnitudes of several mechanical stimuli that are widely considered as candidates to trigger the bone adaptation. A user-material subroutine is developed to relate the magnitude of each candidate to changes in mechanical properties and shape of trabeculae in the baseline model. The obtained adaptation results are qualitatively compared against the follow-up model.

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Microstructure-based modelling of thermomechanical behaviour of cast irons

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Key Words: *Microstructure, Thermal load, Cast iron, RVE, Micromechanics*

Thermomechanical behaviour of cast irons is computationally investigated in this work, employing a micromechanical approach. Cast irons form an integral part of industrial applications, since they are used extensively in numerous applications thanks to their good thermal and mechanical properties, excellent wear resistance, and competitive price [1]. Although cast irons were studied considerably, their thermomechanical behaviour and, especially, fracture at microscale is not yet fully understood. The main reason for this is their complex microstructure comprising graphite particles of different shapes, sizes, and orientations embedded in an iron matrix, which can be pearlitic, ferritic, or a combination of these two phases.

In order to identify the parameters that affect the fracture of cast irons under thermomechanical load, microstructures are characterised with scanning electron microscopy and the obtained scans are assessed with image processing tools. Using statistical analysis of the results, representative volume elements (RVEs) are generated with Python scripts. These comprise a ferritic/pearlitic matrix and graphite particles of various shapes (represented as ellipsoids) and are studied using a finite-element approach. An elastoplastic behaviour is assumed for both graphite inclusions and matrix, while a graphite-matrix interface region is modelled with cohesive finite elements [2, 3]. The focus of this study is on identification of fracture mechanisms at microscale and understanding the macroscopic performance of compacted graphite iron under purely thermal or thermomechanical loading. In addition, parametric analyses are performed to link different microstructural features to mechanical responses. The obtained results are expected to be useful in the future design and optimisation of this engineering alloy and similar metal matrix composites.

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Microstructure-based Thermochemical Ablation Model of C/C Fiber Composites

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Key Words: *C/C composites; Thermochemical ablation model; Microstructure; Ablation recession rate*

The microstructure of carbon fiber-reinforced carbon matrix composites (C/C composites) have important effects on its ablation performance. However, the traditional macro-prediction methods underestimated the ablation recession rate and ignored the influence of microstructure [1, 2]. It is necessary to modify these methods to take the microscopic characteristics into account. Therefore, in this work, a thermochemical ablation model of C/C composites is proposed based on the evolution behavior of its microstructure. The ablation recession rate and surface temperature predicted by this model are in good agreement with the experimental results. Through the numerical analysis, we found that the ablation recession rate of the material without carbon fibers is much greater than that of the material containing carbon fibers. The ablation recession rate is influenced by the fiber orientation due to the change in thermal conductivity. The anti-ablation efficiency of the C/C composites can be improved by increasing its fiber radius, radiation coefficient, heat capacity, interphase density, and thermal conductivity coefficient. The thermochemical ablation model provides a guide for the design of better anti-ablation C/C composites.

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Numerical Modeling of Compression Molded and Shear Enhanced Carbon / Ultra-High-Molecular-Weight-Polyethylene Nanocomposites

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Key Words: *carbon/UHWPE nanocomposites, equal channel angular extrusion, FEA*

Ultra-High Molecular Weight Polyethylene (UHMWPE) is widely used as a bearing surface in total and partial joint arthroplasty. In addition to medical applications, this polymer is utilized in the fields of ballistic protection, sports, and industrial tribology. The addition of carbon allotropes, such as nanographite or carbon black powders, to UHMWPE offers potential benefits including added conductivity, increased wear resistance, and introduction of micro-tracers for understanding microstructural behavior and monitoring damage [1]. The mechanical properties of these carbon/UHWPE nanocomposites can be enhanced by subjecting them to equal channel angular extrusion (ECAE) as a way to introduce large shear strains and achieve higher molecular entanglement of UHMWPE and better distribution of carbon nanoparticles [2, 3].

This paper presents numerical models developed to obtain an insight on the full-field distribution of shear strains during the ECAE process and to correlate the resulting microstructure with the overall mechanical and electrical properties of carbon/UHMWPE nanocomposites. Numerical simulations are conducted on macroscale (ECAE) and microscale (UHMWPE particles and carbon-polymer mixtures) utilizing finite element analysis and analytical micromechanical formulas. The composite material models are based on micro-computed tomography and microscopy studies. Numerical modeling results are correlated with the experimental observations of the extrusion forces and extruded billet shapes (ECAE models) and the overall material properties measurements obtained through thin-section tensile testing (microscale composite models).

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Enhanced Interlaminar Performance and Impact Resistance of Novel Magnesium-based Fiber-Metal Laminates

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Key Words: *Fiber Magnesium Laminates, Interlaminar Performance, Low-velocity Projectile Impact, Constitutive model*

Hybrid carbon fiber reinforced Epoxy (CFRE) composite core/magnesium alloy facesheet laminates are the latest generation of laminates [1]. They have been paid for more and more attention in the fields of electronics, vehicles, aerospace due to their high specific strength and modulus, good shock and energy absorption in comparison to other fiber metal laminates (FMLs). However, the application of the fiber/magnesium laminates is limited because of the weak bonding interface in them. In addition, information on the dynamic mechanical properties of fiber reinforced magnesium-based laminates is very limited [2].

In this work, we focused on the interlaminar performance and impact response of elnov fiber/magnesium alloy laminates (Mg-FMLs) with enhanced interface adhesion [3]. The interlaminar fracture behavior of the Mg-FMLs under different loadings was experimentally studied and the cohesive zone model (CZM) parameters for interfacial bonding layer of the hybrid laminate were extracted by inversion analysis based on the DCB experimental data. Moreover, dynamic response modelling of the FML specimens subjected to low-velocity projectile impact loading was carried out using the developed VUMAT subroutine implemented in ABAQUS/Explicit, and the predicted results were compared to the SHPB experimental results. Results show that the present Mg-FMLs exhibit higher interlaminar fracture toughness and impact resistance than those of traditional Mg-FMLs bonded with epoxy resin [4]. The predicted results for the low-velocity projectile impact are close to the experimental results, validating the correctness of constitutive and finite element models of the composite laminates under dynamic loading conditions. The overall fracture of the present Mg-FMLs under different loading conditions exhibits matrix and CFRP dominated mixed-mode failure because of high interlaminar properties. The research results provide an important reference for the design optimization and application of impact resistant lightweight fiber-metal laminated structures.

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An analytical method for predicting the weathering-induced degradation of slope

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Key Words: *mudstone, cut slope, weathering, rigid-plastic finite element method, infinite slope, Bishop's method*

Weathering-induced deformation of cut slopes excavated in weak rocks is a significant concern for the long-term stability of the slope. In this study, a cut slope at the Tomei expressway was investigated by extensive geotechnical survey and laboratory tests over 50 years to reveal the weathering mechanism after the excavation. From the survey and test results, variation of the stiffness and strength due to weathering was grasped. Interpretation of the safety factor and change in the failure mode due to weathering was predicted by the rigid-plastic finite element method incorporating the strength degradation. A simple, analytical method combining the classical theories of slope stability is developed to predict the weathering-induced change in the safety factor and the failure mode.

15th World Congress on Computational Mechanics (WCCM-XV)
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A 3-D Generalized/eXtended FEM Simulation of Hydraulic Fracture Experiments and Multiple Fracture Interactions

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Key Words: Validation, Generalized FEM, eXtended FEM, Hydraulic Fracture Propagation, Mixed-Mode, *p*-enrichments, Mesh Adaptivity

This work presents a 3-D Generalized/eXtended Finite Element Method (GFEM) simulation of hydraulic fracture process by coupling the solid/rock domain equations with the fluid flow within the fracture using the algorithm reported in [1]. The GFEM, which is based on *p*-hierarchical FEM enrichments, is combined with mesh adaptivity for the robust and computationally efficient simulation of mixed-mode brittle fracture propagation. Both *h*-refinement around the fracture front and *p*-enrichment in the analysis domain are used to control discretization errors. The fluid flow, descritized using a 2-D FEM, is modeled using the Reynold's lubrication theory and assuming a Newtonian fluid property. A Linear Elastic Fracture Mechanics (LEFM) model based on Irwin's criterion is adopted for the solid domain. The direction of fracture propagation is computed using Mode I, II, and III Stress Intensity Factors (SIFs) and Schöllmann's criterion [2]. SIFs are extracted using the Displacement Correlation Method presented in [3]. The formulation cabalities are demonstrated by its adoption to reproduce a set of two hydraulic fracture experimental tests with reasonable accuracy. This is followed by a series of parametric analyses on multiple interacting fractures to study the influence of treatment conditions (fluid viscosity, spacing and number of the fracture cluster and remote stress type) on their behavior.

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A Machine Learning Assisted Multiphysics Model for Reliability Analysis of Underground Pipelines under Environmental Attack

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Key Words: Multiphysics Problems, Random Fields, Hydrogen Environment Assisted Cracking

Past research in stress corrosion cracking (SCC) of pipelines widely relies on expensive and trial-and-error experimental methods to study material susceptibility to cracking under field operating conditions. This work developed a new methodology for using probabilistic multiphysics modeling and simulation of pipelines subjected to near-neutral pH SCC. The mechanism-based hydrogen damage model is solved from a sequence of two stages: colony evolution and cracking. That is, first we predict preliminary stages including time to initiation and starting crack dimensions. Then a second module is used to continue the calculation of the residual strength. Finite element models are validated by existing SCC experiments of X70 steel, with emphasis on the synergistic effects of mechanical and corrosion properties on the material degradation mechanisms. The solution pH and the potential variables are modeled as random fields. Other materials, environment, and stress random variables are considered, and particularly, the initial crack has an aspect ratio modeled from available field data. During uncertainty quantification of the finite element model, an assemble of metamodels is used to alleviate the computational burden of stochastic calculations. The assemble enables a very efficient Monte Carlo simulation, which is performed in the encapsulated algorithm. This surrogate assemble is validated and applied to sensitivity analysis and reliability analysis of the affected pipe. The proposed approach balances high-fidelity modeling with relevant random variables. Furthermore, the proposed approach can reproduce relevant mechanical and corrosion variables that affect stress corrosion crack growth rates. This fact could significantly reduce uncertainties associated with this type of SCC. The results revealed that the probability of failure due to burst is highly sensitive to the crack aspect ratio and toughness due to their influence on crack driving forces. The remaining life can be prolonged greatly by reducing the crack aspect ratio and increasing fracture toughness. In conclusion, it is expected that the presented approach can leads to improvement in the design for reliability of oil and gas pipelines.

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15th World Congress on Computational Mechanics (WCCM-XV)
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A Multi-Resolution Approach to Hydraulic Fracture Simulation

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Key Words: Phase-Field Fracture, Hydraulic Fracture, Multi-Resolution Methods

We present a multi-resolution scheme for simulating hydraulic fracture problems. We consider systems involving a coupling of fluid flow through porous media and within cracks with the mechanics of fracture. In particular, we develop a multi-resolution approach employing a coupling of global and local scales, with distinct treatments in each. Crack propagation is handled inside local subdomains instantiated on the fly in the vicinity of crack tips, using a phase-field method to facilitate the treatment of complex topological changes. The bulk physics are discretized over a global domain, where the fractures are assumed to be fixed and represented by embedded discontinuities. This separation imparts the approach with the benefits of the phase-field method in handling complex crack paths, without requiring the extraction of crack openings from a diffuse crack surface representation. To demonstrate the efficacy of our framework, we compare simulation results using this multi-resolution scheme to well-known benchmark problems in hydraulic fracture, including those with multiple, interacting cracks.

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A PDE-Based Jump Estimation for Phase Field Regularized Cracks

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Key Words: Phase Field, Fracture, Crack Opening, Thermal Contact

Many phase-field formulations for fracture require fast and accurate computation or estimation of jump of quantities across the regularized cracks. For example, the traction-separation law in cohesive fracture, the crack-opening-displacement(COD)-dependent permeability in hydraulic fracture, and the COD-dependent thermal conductivity and the temperature-jump-dependent heat flux in thermal contact all require knowledge about the jump in certain quantities. To date, there have been many attempts at estimating the COD [1, 2, 3, 4, 5, 6]. In this work, we propose a PDE-based approach for estimating general jump quantities across cracks. In the same spirit of phase-field regularization, the jump is first regularized as a density function defined everywhere in the domain. The path-wise constant jump density field can then be obtained from a constrained minimization problem. With prior knowledge about the support of the phase field, a constant jump field over the entire support of the phase field can be recovered. The performance of the proposed method is studied using stationary prescribed cracks and a patch test for thermal contact. Finally, a regularized thermal contact formulation is developed and verified against sharp crack descriptions.

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An adaptive phase-field approach to model failure in orthotropic materials

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Key Words: *phase-field, fracture propagation, damage, composites, orthotropic materials*

Modern day composites have many potential applications in the production of structural components like fuselage, fairings, wing structures etc., as they possess high strength and stiffness-to-weight ratio. The structural components also require fewer fastening and machining parts. Despite the significant advantages of composites, several questions pertaining to the mechanical/failure behavior of composites remain unresolved. For instance, wing structures in aircrafts often withstand high lift and drag forces. Any composite material used in designing these components must withstand these forces without a significant risk of failure. The development of predictive numerical models is thus essential while understanding the failure behavior of composites. However, existing methods fail to accurately predict the various failure mechanisms, such as crack deflection, coalescence, and matrix cracking at the laminate interfaces. Here, we propose the use of an adaptive phase-field approach to address this class of problems.

We extend a recently developed adaptive phase-field method to model delamination in orthotropic laminated composites [1]. In the proposed approach, two sets of governing equations are simultaneously solved in a staggered manner. A second-order partial differential equation is solved to obtain a phase-field variable that predicts the damage evolution. A coupling between the mechanical equilibrium equations and the phase-field damage variable equation is achieved through a stress-degradation function. The dependence of the crack path on material orientation is incorporated by means of a penalized second order structural tensor in the crack surface density function [2]. Crack driving force was divided into individual fibre and matrix damage, corresponding to different failure modes across laminate [3]. An adaptive refinement strategy is finally suggested, to reduce the computational cost, that robustly discretizes the domain as the crack propagates. The computational mesh is partitioned into standard and refined regions, which is mapped onto a fixed background mesh with different approximation spaces. A continuous finite element approximation is used while partitioning the regions, weak continuity is then imposed at the interface using Nitsche's method. Benchmark numerical experiments were performed to demonstrate the efficacy of the approach to capture failure behavior in composite laminate by varying fibre orientation. Results exhibit the great capability of model to predict crack propagation which was either along the interface or it cuts the matrix. The numerical findings were validated by existing experimental and numerical studies.

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Numerical modeling of fracture propagation in layered materials using an adaptively refined phase-field method

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Key Words: *phase-field, fracture propagation, layered media, subsurface fracture*

Fracture propagation in layered subsurface media is actively studied by engineers, and geoscientists. In various geo-engineered systems, such as, unconventional hydrocarbon reservoirs, enhanced geothermal systems, tunnels, and mines, fracture patterns in the subsurface play a critical role. Predictive numerical simulations are an essential tool to facilitate well-designed subsurface systems. However, despite significant advances in recent years, numerically predicting fracture propagation in the subsurface remains an outstanding challenge for the computational mechanics community. This is partly because the subsurface is highly heterogeneous and contains several layers with distinct mechanical properties, which dramatically affects the geometry of subsurface fractures. Depending on prevailing conditions of contrasts in elastic moduli, fracture toughness, interface inclination, and in-situ stress of surrounding layers, cracks may either arrest, penetrate, or branch at the material interface [1].

This study will extend a recently developed adaptive phase-field fracture model to layered materials [2]. In this approach, mesh refinement is required only in a small, diffused zone ahead of the crack tip while the rest of the domain is discretized using standard elements. The continuity between refined and standard elements is ensured by employing the Nitsche's method. The key advantages of the proposed methodology include an energetic approach to the crack propagation criteria, a natural crack-tracking framework through a phase-field variable, and reduced computational burden due to mesh adaptivity. Several parametric studies will be performed to study the effect of elastic stiffness contrast, toughness contrast, and interface inclination on fracture propagation in layered subsurface formations with perfectly bonded layer interfaces. Based on these studies, conclusions will be drawn on the conditions that result in fracture arrest, deflection, and penetration at layer interfaces in multi-layered formations.

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Phase-field modelling of fracture behavior of heterogeneous random porous materials

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Key Words: *Fracture phase-field model, One-cut Gaussian random field, Sintered silver nanoparticles*

Nowadays, sintered silver nanoparticles, a promising candidate for electronics interconnection materials, are widely adopted in emerging electronics technologies such as next-generation power electronics, polymeric devices, skin-mounted device, printable elastic conductors, and wearable printed circuits. Owing to its low sintering temperature, high melting point, and excellent thermal and electrical conductivities, sintered silver nanoparticles allow reliable electrical and mechanical interconnects to be used for various substrates and harsh environments. Essentially, sintered silver nanoparticles are typically heterogeneous with randomly distributed pores are ubiquitous.

Recent experimental investigations have revealed that porosity and also the pore-related geometries (size, number, shape, distribution and alignment) have significant impacts on the mechanical behaviour of random porous materials. However, existing studies focus on the porosity effect while ignoring other pore features such as pore size and pore shape. Our research is dedicated to a computational framework for generating isotropic/anisotropic random porous materials using Gaussian random fields with stochastic pore size and shape factor and addressing the mechanical properties and behaviour of brittle fractures using a fracture phase-field model with a preferred degradation function. Sintered silver nanoparticles with typical randomly distributed pores, as representative porous materials, are chosen for their promising applications in emerging fields such as power electronics and wearable devices. In order to emphasize the effect of pore size and shape, 420 random samples with a fixed porosity were generated to discuss the stress-strain response during fracture and to establish statistical relationships between pore feature distributions and mechanical properties such as Young's modulus, UTS, and average historical energy. Our findings suggest that the statical attributes of the pore sizes and shape factors significantly affect the material performance related to the mechanical properties and fracture behaviour, which could give a better understanding of the random porous materials and guide reliability-based material design and optimization.

Further studies can be done in the future to expand into the three-dimensional structure in order to gain a better understanding of the correlation of true microstructure with mechanical behavior. The relationship between three-dimensional spatial distribution features and mechanical properties can be investigated for random porous structures as well. On the other hand, a huge number of random samples generated by our approach can be studied more effectively by machine learning. Efficient and fast links between random porous structure and mechanical characteristics can be developed by machine learning, which can drastically reduce computational consumption and achieve microstructure-based material attributes more quickly.

Updated-Lagrangian XFEM Formulation for Ductile Fracture at Large Strain

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Key Words: *Ductile Fracture, Finite Strain, X-FEM, Updated-Lagrangian Formulation*

The numerical treatment of the whole process of ductile fracture remains a challenging task, particularly when FEM is employed. The well-known main issue regards pathological mesh dependence of the numerical results, not only in the softening regime induced by the more or less diffuse micro-defect growth, but also in the stages of strain localization and further crack propagation that are strongly controlled by the mesh size and orientation and not by physics. In the literature, non-local approaches are adopted to mitigate these effects but they require a calibrated length scale and mesh refinement, thus being time consuming. In order to get both mesh objectivity and low computation cost, we here propose to apply the XFEM to both weak and strong discontinuities, viz. strain localization and crack propagation. A three-dimensional methodology assuming small strain has been implemented into the commercial code Abaqus through a user-element (UEL), wherein the strain localization band is described through a cohesive plane embedded within the finite element (cohesive XFE), and the progressive loss of cohesion leads to crack formation (traction-free XFE), see [1]. We further extend this methodology considering large strain and rotation, relying upon the Updated Lagrangian formulation (U.L.) (see [2]), incrementally objective algorithms as proposed in [3], and various cohesive models. The main numerical issues, such as locking (see [4]) that were necessary to solve/overcome will be presented along with cases of increasing complexity (geometry, loading). A final assessment of the numerical approach implemented in Abaqus will be conducted by comparing numerical results to experimental results.

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3D X-FEM Modeling of Crack Coalescence Phenomena in the Smart-Cut Process

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Key Words: X-FEM, coalescence, Smart Cut, SOI, SIF

It has been shown that the coalescence of pressurized penny-shape cracks leads to controlled fracture of silicon which is the basis of Smart-Cut process used to fabricate silicon on insulator (SOI) wafers [1]. In this study, we report the results of the simulation of multiple crack evolution and their coalescence using the eXtended Finite Elements Method (X-FEM). This approach can offer accurate and optimally convergent numerical solution of elastic fields using level sets functions and enrichment technique to define a crack [2]. We have addressed the problem with a 3D model and in linear elastic fracture mechanics framework. A multi-scale adaptive mesh has been developed in the form of 3D fractal mesh to optimize computation time. About 90% gain in computation time has been achieved compared to structured meshes. Neumann boundary conditions for pressure have been applied on crack interfaces. This type of load represents pressure in cavities produced by hydrogen gas created by H implantation followed by annealing during Smart-Cut process. Another contribution of this study is related to the determination of 3D stress intensity factors (SIF) with internal pressure applied on crack interfaces. Numerical results on SIF K_I have been compared to the analytical solution in the model case of isolated round penny-shape crack in equilibrium, demonstrating very good accuracy (less than 1%). The crack growth is taken into account in the model following Griffith's theory for brittle fracture [3]. The coalescence modeling has been possible by updating level sets and enrichments at the crack vicinity. The final challenge in this study is the modeling of experimentally observed cracks evolution [1] to explain physical aspects of cracks in the Smart-Cut process and to evaluate local instabilities related to crack size and shape.

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A peridynamic fatigue model based on two-parameter remaining-life formulation

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Key Words: *peridynamic fatigue model, remaining-life, crack driving force, R-ratio effect*

The peridynamic fatigue model using the remaining-life concept was developed by Silling and Askari [1]. In this model, fatigue damage induced by cyclic loadings can be simulated by applying the remaining-life solution as a failure criterion. Herein, the remaining-life solution is based on only the single parameter of the core cyclic bond strain induced by cyclic loadings. Bang et al. [2] and Bang and Ince [3] showed that the model has a limitation of accounting for fatigue damage induced by both monotonic and cyclic loadings, i.e., effects of R-ratio are not considered in the peridynamic fatigue damage model.

To overcome this problem, a new peridynamic fatigue model based on two-parameter based remaining-life concept is proposed in order to take into account R-ratio effects in peridynamic crack growth simulations. Two-parameter remaining-life equation is formulated as a function of the core cyclic bond strain and maximum core bond strain considering two-parameter nature of fatigue damage process. The core cyclic bond strain and maximum core bond strain are regarded as two independent peridynamic crack driving forces in a new formulation of the PD fatigue damage model. The proposed model provides a capability that more accurate crack growth simulations can be obtained by accounting for two independent damage controlling parameters of the core cyclic bond strain and maximum core bond strain resulted from the cyclic and monotonic parts of a loading cycle, respectively.

The model results show the predicted crack growth rates computed by the model agree well with experimental data set of 2024-T3 and 7075-T6 aluminium alloys under four different R-ratio loading conditions of $R = 0$, $R = 0.33$, $R = 0.5$ and $R = 0.7$. The model predictions also show that two-parameter based crack growth driving force enables crack growth data sets at various loading conditions are collapsed on the predictive master curve of the model. The proposed peridynamic fatigue damage modeling approach provides efficient and accurate crack growth simulations by accounting for different R-ratio loading conditions. The unification of fatigue damage behavior under various cyclic loading conditions can be possible by accounting for two peridynamic damage controlling parameters of the core cyclic bond strain and maximum core bond strain in the formulation of the fatigue damage model on the basis of two-parameter based remaining-life formulation.

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A unified nonlocal model for capturing discontinuous, multiphysical and multiscale behaviours of geomaterials

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Key Words: *Peridynamic, Multiphysics, Multiscale, Discontinuous, Geomaterials*

A unified peridynamic model (UPD) is proposed to simulate the discontinuous, multiphysical and multiscale behaviours of geomaterials. The mechanical behaviours of the material points are reformulated by incorporating the bond tension-rotation-shear coupling effects, which makes the proposed model suitable for complex discontinuous problems in both three-dimensional spatial and two-dimensional plane conditions. The governing equations of bonds connecting material points are reformulated from the definition of bond deformation rates, leading to a rate-based expression of mechanical behaviour of solid particles. Three kinds of peridynamic parameters, corresponding to the compressive, shear and bending stiffness of the bond, are introduced to keep the consistence of the strain energy obtained from the proposed peridynamic model and from the continuum mechanics under arbitrary deformation fields. The damage evolution functions are introduced in the model to capture the loading-rate dependence of geomaterials. Moreover, a novel energy-based failure criterion, involving the maximum stretch, shear strain and rotation angle limits of the bond, is proposed to describe the nonlinear behaviors and progressive failure for geomaterials.

In order to further simulate the continuous and discontinuous mechanical behaviours of geomaterials under effects of different physical fields, a nonlocal multiphysics model is proposed in the framework of the UPD. A new force state vector is proposed by introducing the first Piola-Kirchhoff stress to enable the divergence of stress tensor at each material point to be expressed by averaging all the force state vectors in its support domain. It is also demonstrated that the new force state vector ensures the mathematical consistency between the strong form of peridynamic (PD) and the classical continuum mechanics (CCM) when the horizon of a material point approaches to zero. Then, a non-local Gauss's formulation is presented by transforming the displacement and traction boundaries in CCM into the non-local fictious boundary layers in PD, and this formulation unifies the variational framework of PD and CCM at both continuous and discrete levels. Furthermore, a fully implicit algorithm is developed to solve the general nonlinear problems such as fracture behaviours and large deformation of solid materials. Fianlly, a penalty method is employed to eliminate the zero-energy mode oscillation inherently observed in NOSB-PD, and the penalty force and penalty stiffness matrix are derived in the proposed implicit algorithm and numerical implementation.

To modelling the mechanical behaviours of the fluid transport in porous media, a unified non-local fluid transport model is developed along with the idea of UPD. First, a non-local governing equation of fluid transport is presented based on the UPD, and a novel flux vector state and a non-local Darcy's law is proposed to illustrate non-local fluid transport effects in heterogeneous saturated porous media. The proposed flux state vector ensures the non-local governing equation of fluid transport model in heterogeneous saturated porous media degenerates into the local one when the horizon of each material point approaches to zero. A non-local pressure gradient at each material point can be obtained by averaging all the flux state vectors in its horizon, which unifies the weak and strong discontinuities of pressure in heterogeneous saturated porous media in a consistent way. Second, a variational formulation of the unified non-local fluid transport model is developed. This variational formulation enables the proposed model to deal with complex boundary conditions, which is difficult or even impossible for current fluid transport models

based on Bond-based Peridynamics (BB-PD) and Ordinary State-based Peridynamics (OSB-PD). Third, a fully implicit algorithm combined with the Newton-Raphson method is introduced to solve the general non-linear problems in the heterogeneous saturated porous media.

For the simulation of multiscale behaviours of geomaterials, the PD model based on nonlocal theory is coupled with the finite element method (FEM) based on classical continuum mechanics, which can eliminate the boundary effects caused by nonlocal effects. The PD and FEM models are coupled by the hybrid region, which is based on the simplified energy equivalent method. In the hybrid region, there are three kinds of transition weight function: Heaviside function, linear function, and cubic function. The dynamic relaxation method is used to reach a solution. The computational accuracy of the coupling method with different transition weight functions is verified by comparing the results of numerical examples with the FEM results. The coupling method lays a foundation for multi-scale discontinuity problems.

The proposed model is verified by comparing its results with those from experimental observations. Numerical examples demonstrate that discontinuous, multiphysical and multiscale behaviours of geomaterials under dynamic loads are well captured by the proposed model.

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Data-Driven Mechanics for Non-Local Solid Mechanics with Frankenstein's Method

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Key Words: Computational Solid Mechanics, Data-Driven Mechanics, Non-Local Models

A new data-driven method for solid mechanics is proposed. The fundamental idea is to use full field displacement measurements to obtain admissible solutions over larger domains, called patches. As these patches have been observed in real structures, they automatically meet most of the PDE characterizing the problem, especially internal equilibrium and constitutive equation. We then use a library of such patches to predict the response of new structures. To do so, patches are assembled as pieces of a jigsaw puzzle in a way that they meet the boundary conditions exactly while they meet some globally defined approximation of equilibrium and kinematic continuity. No assumption on the locality of the problem was made, as the objective of the method is to be model-free. For this purpose we use an overlapping domain decomposition method that is applicable to both local and non-local problems.

Frankenstein's method can be readily applied to non-local problem without much additional complexity compared to local formulation, as it is by essence formulated independently of the locality/non-locality assumptions. This should allow for a more natural implementation of plasticity, degradation and damage in the future, as these are commonly accompanied by localization issues [1]. One can also see this work as an extension of non-local methods. The accuracy of traditional non-local models such as peridynamics, phase-field or higher order gradient methods, depends upon the formulation of an accurate constitutive relation. But traditionally constitutive relations are found empirically, the choice of a material model is essentially arbitrary, one simply decides on a fit function which seems appropriate as long as some thermodynamic principles are satisfied [2]. Our work does not require such a heuristic approach, it is a first effort towards a uniform framework. Removing the heuristics comes with a price however, an increase of computation cost and measurement data hunger.

We will introduce the fundamentals of Frankenstein's Method illustrated by history independent examples in one and two dimensions. The main focus is the formulation of a weak form, which will allow for the approximation of the exact solution.

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Dynamic Fracture in Glassy Polymers: Peridynamic Models

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Key Words: *Peridynamics, Dynamic Fracture, Glass, PMMA, Interfaces, Fracture Process Zone*

Peridynamic (PD) models for dynamic brittle fracture have been shown to predict complex crack patterns, the crack speed, and interactions between stress waves and propagating cracks. The models have been validated against experimental results for dynamic crack growth in glass [1,2]. There is also a clear understanding why, in contrast, phase-field models have difficulties in matching some of the experimentally observed behaviour. Nevertheless, when the PD models for brittle fracture are applied to certain glassy polymers (e.g. PMMA), they lead to crack propagation speeds significantly higher than what is measured in experiments. We investigated the reasons behind these discrepancies and found that the likely culprit is softening due to heating near the crack tip: experimental evidence has been published showing significant heating/melting around the process zone in dynamic fracture in PMMA materials. We concluded that heat generated by high strain rates at the crack tip, or its softening effects, need to be taken into account if one aims of predicting dynamic fracture in PMMA.

We introduced a PD model ([3]) that implements a Heat Affected Zone (HAZ) around the crack tip in which a nonlinear (bilinear) elastic model is used before peridynamic bonds break, in order to affect the softening due to heat generation from high strain rates. The model with a softened region around the crack tip was able to reproduce the experimentally measured crack speed and the crack length evolution with high fidelity. The new peridynamic model allowed us to understand the relevant mechanisms in dynamic fracture of PMMA. With this model, we demonstrated the importance of the softened region around the crack tip in dynamic fracture of PMMA materials.

The model was then used to study the influence of strong and weak interfaces in bi-layered PMMA on crack behaviour [4]. Experiments have shown that PMMA layers exhibit dramatic changes in dynamic crack growth characteristics depending on the interface toughness and its location. We find that the presence of three factors/elements in the PD model are essential for being able to reproduce the observed fracture behaviour: (1) softening near the crack tip to account for changes in PMMA due to heat-generation induced by the high strain rates reached around the crack tip in dynamic fracture; (2) having independent extension (mode I) and shear (mode II) modes of fracture; and (3) using a two-parameter fracture model (that can match both the strength and the fracture toughness for any horizon size). Once these elements are in place, the PD model captures the experimentally observed dynamic fracture characteristics in bi-layer PMMA: cracks branching or not at the interface, depending on the interface location; crack running along the interface and punching through the second PMMA layer; slight crack path oscillations near the far end of the sample. The computed crack speed profiles are also close to those measured experimentally. The model reproduces the slight crack acceleration seen before the crack tip reaches the interface, and the sudden drop in crack speed once passed the interface.

We conclude that dynamic brittle fracture models for PMMA require extra components compared to those that work for dynamic fracture in glass, for example. Moreover, the presence of interfaces constitutes an important benchmark against which computational models for dynamic

fracture need to be tested against: a model can perform well when simulating dynamic brittle fracture in a homogeneous sample, but fail when the sample is simply a layered construct of the same material.

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Employing a Bézier curve model for simulating microstructure generation during the additive manufacturing process to inform microstructure aware material models

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Key Words: additive manufacturing, peridynamics, microstructure aware model

The microstructures of additively manufactured materials are spatially heterogeneous and highly process dependent. Moreover, engineering properties such as strength and toughness are sensitive to microstructure morphologies resulting from the manufacturing process. The creation of microstructure aware material models, in fields such as peridynamics [1], requires data describing the underlying microstructure.

This presentation will discuss recent work on a model employing the Metropolis Monte Carlo method for simulating additively manufactured microstructures. The proposed model allows flexibility in the process parameters which facilitates the analysis of the impact of process parameters on the generated microstructure. This model is implemented into the open source code SPPARKS [2].

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Fracture analysis of bimaterial interface with the residual thermal deformation by peridynamic model

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Key Words: *Peridynamics, Bimaterial fracture, Residual thermal deformation, Interface delamination*

In this work, the role of residual thermal deformation on bimaterial interface fracture is investigated by the peridynamic model. First, the formation of peridynamic bond force state considering thermal effect is given for the bimaterial elastic behaviours modeling. The energy release rate of bimaterial interface crack with the thermal deformation is computed with the modified peridynamics-based virtual crack closure technique (PD_VCCT) model. An extended peridynamic mixed-mode bond failure model considering thermal effect is proposed for interface bond failure analysis, and a node to node peridynamic contact model is introduced for the frictional contact modeling of interface cracks. Then, some examples are investigated for the model verification and application. The deformation and fracture behaviours of bimaterial specimens are predicted with the proposed peridynamic models, and the role of residual thermal deformation is studied.

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Quasistatic Fracture using Nonliner-Nonlocal Elastostatics with an Analytic Tangent Stiffness Matrix for arbitrary Poisson ratios

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Key Words: Quasistatic fracture, nonlinear-nonlocal elastostatics, hard and soft loading

We use nonlinear-nonlocal field theory for numerical simulations of quasistatic fracture. The model used is a regularized nonlinear pair-wise (RNP) potential within the peridynamic formulation. In addition, to the tensile force, a hydro force is added to allow arbitrary Poisson ratio. The potential functions are analytic and smooth. This fact allows us to write the entries of the tangent stiffness matrix analytically thereby saving computational costs during the assembly of the tangent stiffness matrix. We validate our approach against some state-based peridynamic model using numerical differentiation for the tangent stiffness matrix and classical continuum mechanics. In addition, we show stable crack growth for hard loading. Our approach is novel in that only bond softening is used, as opposed to bond breaking.

Study on thermal fatigue of nickel-based superalloy composites using Peridynamics method

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Key Words: *Superalloy Composites, Peri-Dynamics, Thermal Fatigue, Damage,*

Nickel-based superalloy is a metal composite material with nickel as matrix and reinforcement. It has high strength and resistance to oxidation and corrosion at high temperatures, and has a wide range of applications in the fields of transportation, aerospace and energy. Experimental research on fatigue-resistance performance of nickel-based superalloys in high-temperature extreme environments has disadvantages such as complex experimental procedures, high research costs, and low efficiency. Herein, a temperature-dependent fatigue crack growth model of conventional peri-dynamics（PD）was established to simulate the fatigue crack growth behavior of graphene/nickel-based superalloy composites under thermal cyclic loadings. The effects of thermal cycle amplitude and graphene content on the thermal fatigue crack growth behavior of the superalloy composites are studied. The PD method describes the damage behavior of composite materials by solving the spatial integral equation, which effectively avoids the singular solution of the damage simulation crack, and the simulation calculation accuracy of the thermal fatigue crack growth behavior of the material is high. The present PD model provides a new idea for the numerical study of mechanical behavior of metal composites under extreme environment.

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A discrete slip plane model and its application to experiments on ferritic mono- and polycrystals

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Key Words: Crystal Plasticity, Dislocation Sources, Stochastics, Ferrite

Micro-scale mechanical tests, such as micropillar compression tests or microtensile tests, play an important role in understanding the mechanical behavior of metals. Complementing these experiments by simulations can give additional insights into the observed behavior and allows for predicting the behavior in polycrystals. However, traditional crystal plasticity models fail to capture the heterogeneous deformation within a single crystal and the variations in the stress-strain curves between similar samples that are observed in experiments. These stochastic variations arise because of the limited number of dislocation sources present in the samples. On the other hand, simulation frameworks which do account for the stochastics of dislocation sources, such as discrete dislocation dynamics, come with significant computational cost and complexity and are often restricted to small displacements. This impedes the application of these simulation frameworks to full microscale experiments.

We present a numerical framework [1] which models the plastic deformation resulting from slip on crystallographic slip systems, similar to the approach taken in crystal plasticity, but which does account for variations in critically resolved shear stresses between atomic planes. These variations are linked to the physics and stochastics of dislocation sources. By using some verified assumptions, only small adaptions to a standard crystal plasticity code are needed in order to implement the model. This allows for simulations up to large strains, in a finite deformation setting. The numerical framework is used to study the behavior of microtensile tests of ferrite monocrystals, performed by Du et al. [2]. It is shown that the discrete slip plane model, contrary to a traditional crystal plasticity model, is able to predict the diversity of active slip systems, the heterogeneous deformation and the variations in the stress-strain curves that are observed in the experiments. Furthermore, the model is applied to samples consisting of multiple grains. Here, the competition between stochastic effects and microstructural features is studied.

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A Hyperbolic Phase Field Model for High Strain Rate Fracture in Microstructured Media

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Key Words: *Phase Field, Microstructured Media, Rate Effect*

Continuum damage models that possess an internal length scale address the mesh sensitivity of earlier damage models wherein the response becomes more brittle as the mesh is refined. However, in many applications the crack-tip damaging zones for propagating cracks tend to be overly diffuse and broad. While the phase field formulation derives from a different energy statement, the final form of differential equation resembles a gradient damage model, albeit with some differences in the source term and stress reduction function. These differences improve the phase field model response by reducing diffusion in damaged regions.

We consider the elastodynamics problem coupled with a hyperbolic phase field model. The rationale for using a hyperbolic phase field model is the finite speed of propagation of waves and damage in solid materials. This argument motivates the phase field model in [1] and the continuum damage models in [2, 3]. We present elliptic, parabolic, and damped hyperbolic forms of phase field differential equations and describe the interaction between the phase-field time scales (where present) and the time scale of dynamic loading in a 1D problem. The rate effects of the phase field models will also be compared with a continuum damage model. Understanding the induced material rate effects based on intrinsic parameters of the phase field model is important for extending the model to more complex 2D and 3D problems. Next, the asynchronous spacetime discontinuous Galerkin (aSDG) method [4] is used for 2D solutions. Specifically, the failure response of microstructured media composed of repeating unit cells is sought. The metamaterial microstructure is designed to delay the transfer of energy and to decay stress amplitude as waves pass through a slab of material. Finally, we briefly discuss applications of this accurate but computationally expensive continuum model for fine-tuning the parameters of extreme reduced order models (ROMs) based on discrete representations of grids of metamaterial cells.

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A New Energy Limiter-based Damage Approach for Brittle Fracture

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Key Words: *Brittle fracture, Energy limiter, Crack band theory, Energy decomposition, FEM*

We present a new scalar damage model for brittle fracture under quasi-static and dynamic loading conditions in both 2D and 3D problems. In contrast to existing damage theories, the new development is derived in the context of scalar damage theory, but the damage variable is defined by means of the energy limiter theory [1] with an introduction of the damage threshold. The model is further enhanced with crack band theory [2] and energy decomposition [3]. Finite element discretization for the developed approach at small strain for localized brittle fracture is given. The developed damage model consists of three major ingredients: (i) the energy limiter theory is introduced as the foundation of the developed formulation; (ii) the crack band theory is to regularize the formulation to avoid mesh-dependent solutions; (iii) the split energy density uses to differentiate fracture behavior between tension and compression modes, preventing the non-physical crack in compression domains. We present several representative numerical examples to show the performance and accuracy of the developed damage model.

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Consistent Description by Cohesive Traction-Separation Law for Seamless Transition from Weak- in Strong-Discontinuities

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Key Words: Cohesive Zone Model, Damage Model, Micromorphic Approach, Crack Propagation Analysis

This study present a consistent description of the cohesive traction-separation law for seamless transition from weak- into strong-discontinuities. The fracture process can be divided into two stages to differentiate discontinuities in the displacement field around a crack tip. At the first stage of the fracture process, the displacement field changes from continuous to weakly-discontinuous ones due to the pseudo-jump discontinuity of the strain field caused by the stiffness reduction followed by material softening. The stiffness reduction is represented by the cohesive traction-separation law that is incorporated into a material constitutive law by the introduction of apparent strain caused by the crack opening displacement and the local balance equation between cohesive traction and principal stress. Moreover, we employ the micromorphic approach [2] that allows us to connect between microscopic variables representing apparent strain at local material points and micromorphic variables corresponding to that at global domain. As a result, the transition of the displacement field from continuous to weakly-discontinuous ones is realized by diffusive approximation. At the second stage, the displacement field is developed into jump discontinuity, as it is called the strong discontinuity by an explicit crack opening along with the material softening behavior. To realize a discrete crack opening, a finite cover method (FCM) [3] is employed by the combined use of the cohesive traction-separation law. The same cohesive traction-separation law is applied to keep consistent description between these two stages of the fracture process. The capability of the proposed method is demonstrated through several numerical examples.

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Damage regularization via the Eikonal gradient non-local method: properties and couplings with plasticity

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Key Words: Damage mechanics, gradient regularization, non-local model

While damage mechanical models have been developed for decades now, the transition from diffuse degradation to a single fracture zone still remains a difficulty. Indeed, beyond a certain loading level, damage models generally lead to localized solutions of the associated continuum mechanics problem. The localized area corresponds to a crack but, without regularization, the problem becomes ill-posed, which results into spurious mesh dependency, e.g., the dissipated energy tends to zero as the finite element size tends to zero. Various solutions have been proposed in the literature [1], relying on a spatial non-local treatment of the regularization. The driving forces are averaged to introduce an internal length that enforces mesh independency. The averaging can be conducted directly or through an auxiliary boundary value problem. The internal length may be constant, in which case all interactions are not cut by a fully damaged zone, or the internal length can evolve with stress to account for boundary conditions and cut the interactions across a crack.

The aim of this paper is to present a non-local gradient regularization technique called the Eikonal non-local gradient model [2]. It is a gradient regularization which replaces the classical internal length by a varying metric originating from the acoustic wave speed. The potentially anisotropic metric evolves with damage, as in phase-field models, thus cutting interactions when the damage reaches one. The first part of the contribution presents this model and the associated properties on a 1D problem in tension. A comparison to other classical methods is also given. This example shows the good behavior of this regularization technique. It is shown that the evolving characteristic length leads to a rather sharp and brittle post-peak behavior. A plasticity model is then coupled to damage in order to decrease the brittleness of the mechanical response. This choice is illustrated to better understand the interactions between damage, regularization and plasticity.

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Entropy-based damage model for fatigue behaviour of lead-free solder materials

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Key Words: *Entropy-Generation; Damage Model; Fatigue Behaviour.*

Solder materials are playing an increasingly important role in the electronic packaging structures in the development of electronic products. The mechanical reliability of packaging structures is directly related to the service life of the entire device or system, especially under harsh application conditions. In view of the fact that the CTE varies greatly for different materials in the package structure, the deformation of the packaging structure due to temperature change during thermal cycling will lead to mismatched thermoelastic deformation and stress concentration between different materials. Thereafter, selecting and describing the mechanical properties of solder materials has become crucial from the practical viewpoint.

In order to describe the influence of damage accumulation on the structural properties of the packaging material under the effect of cyclic loaded thermal mismatch, low cycle fatigue experiments were performed in the present study on Sn-3.0Ag-0.5Cu (SAC305) specimens at a strain level of 0.12 subjected to different temperatures and different strain rates. Based on the Newtonian mechanics and the thermodynamic theory, the entropy generation was derived as a damage parameter. Combined with the strength degradation under different cyclic loading conditions, the other parameters are determined to be related with the damage parameter. The relationship between the number of cycles and the peak stress for 400 loading cycles at various temperatures and a strain amplitude of 0.01. Apparently, the applied 400 strain cycles in this study are sufficient to result in the evolution and also the stabilization of peak stress for SAC lead-free solder materials. After comparing the peak stress at different temperatures, it can be found that SAC305 exhibits obvious temperature softening phenomenon, as its peak stress decreases as the number of cycles increases. Eventually, the damage evolution is proposed by correlating with temperature and strain rate, which to our knowledge has never been realized before for lead-free solder materials. By expressing the entropy generation as a function of variables such as stress tensor, plastic strain and temperature, the proposed damage factor comprehensively covers the influence of plastic work, thermal loading and other loading factors. In accordance with the quantitative law that fatigue entropy increases with the number of cyclic loading during fatigue deformation, the damage evolution law during temperature cycling is determined, thus establishing a damage-entropy generation model for packaging materials, which can reasonably describe the evolution law of accumulated damage of solder joints. In order to further elucidate the microscopic evolution of SAC305 under different cyclic conditions, the microstructure of SAC305 after fatigue tests was also examined by a scanning electron microscope (SEM).

Fracture of A neo-Hookean Sheet: An Arc-Length Method-Based Phase Field Model and Crack Tip Fields

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Abstract: In this talk, we present damage effects on the crack tip fields in a neo-Hookean sheet based on a phase field model. We first introduce 1D and 2D phase field models which are able to track non-monotonic evolution of the equilibrium paths in facture process. In the incremental governing equations, a supplementary arc-length equation is introduced and consistent stiffness matrices are implemented [1]. The snap-back phenomena in fracture of a 1D bar and a 2D notched long strip are captured. We calibrate the material parameters using an energy based approach. We observe good agreement between the simulation and the experiment for the 2D notched strip in different loading cases [2] using only a single set of calibrated parameters. Based on the results of the phase field models, we derive asymptotic crack tip fields of a neo-Hookean sheet with prescribed distribution of the material damage. The features for the crack tip fields with the effect of material damage are summarized. We observe that the crack tip fields at the crack front are similar when the crack advances. The stress field shows a peak value in the front of crack and decreases to zero as the distance to the new crack tip goes to zero, rather than shows the singular behavior observed in results based on pure hyperelasticity [3,4]. Also, due to the presence of material damage, the stress near the crack faces is significantly reduced. These results provide new insights in understanding fracture mechanism for hyperelastic materials in the area of soft robotics and biological tissue.

Key Words: *crack tip fields; neo-Hookean materials; phase field model; asymptotic analysis; finite element method*

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Highly Anisotropic Plasticity of Lath Martensite – Computational Modelling and Comparison with Experiments

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Key Words: computational micromechanics, crystal plasticity, experimental characterisation, advanced high strength steel

Advanced high strength steel grades based on dual phase or complex phase microstructures employ carefully designed mixtures of hard and soft phases to achieve a strong and ductile effective material response. Among these phases, lath martensite is the hardest and its role is thus to provide strength to the system. At the same time, it is quite brittle, hence limiting the overall ductility of the material. However, there is an increasing amount of experimental evidence of large plastic strains occurring in lath martensite [1]. They tend to occur in grains which are oriented such that the inter-lath boundaries experience a high shear stress. It has therefore been hypothesised that the plastic deformation occurs in thin (nm scale) retained austenite films, trapped between the laths, which by virtue of the orientation relationships always have slip systems parallel to the lath boundaries [2]. Developing a deeper understanding of this phenomenon is of practical relevance because it may provide a pathway to improve the ductility of the material at no (or limited) cost in terms of loss of strength.

Our objective in this study is to formulate an aggregated model for lath martensite plasticity, based on the hypothesis of pronounced slip in interlath retained austenite films, and compare predictions made by microstructural simulations based on the model with microscale experimental observations on a dual phase steel grade. The modelling targets the level of individual packets. It is founded on a full, conventional BCC crystal plasticity representation of the laths within the packet. The additional plastic deformation model facilitated by the austenite films is accounted for by adding (only) the three FCC slip systems parallel to the habit plane (and thus to the interlath boundaries) to the crystal plasticity description. Combining the resulting model with conventional crystal plasticity for ferrite allows us to capture the plastic activity distribution observed experimentally in dual phase microstructures.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Implementing Nonlocal Ductile Damage Into a Large Strain FFT-Based Model for Predicting Failure in Polycrystalline Materials

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Key Words: Ductility, Crystal Plasticity, Continuum Damage Mechanics, Fast Fourier Transform

Ductility is an important property that describes the amount of macroscopic deformation a material can endure before failure. Ductility can vary significantly based on geometric or microstructural size effects, especially at sub-millimeter length scales. Many previously developed finite element (FE)-based crystal plasticity models incorporate porous plasticity or continuum damage mechanics (CDM) to predict ductile failure. However, such FE models require significant computational resources. Fast Fourier transform (FFT)-based models are a growing alternative to FE-based models as they can accurately predict micromechanical fields at a fraction of the cost of traditional FE models. Several previously developed FFT-based models have incorporated either crystal plasticity or CDM; however, there remains a need to couple both methods together to predict ductile failure in polycrystalline materials. Using an FFT-based crystal plasticity method, we explore the effects of specimen geometry and microstructure on macroscopic ductility. This work incorporates a nonlocal triaxiality-based CDM formulation into a large-strain elasto-viscoplastic fast Fourier transform (LS-EVPFFT) model [1] to predict ductile failure in polycrystalline microtensile copper coupons. Simulations with the damage-enabled LS-EVPFFT model are compared to the macroscopic and micromechanical response from copper microtensile specimens characterized with electron backscatter diffraction (EBSD) and in situ digital image correlation (DIC). The low computational cost of the damage-enabled LS-EVPFFT model allows for the macroscopic ductility and ductile failure location of polycrystalline materials to be tractably predicted. This work is part of a continuing effort to develop models that accurately represent the entire elastic-plastic-failure loading process of complex 3D polycrystalline materials while retaining low computational cost.

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Lipschitz Regularization For Softening Material

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Key Words: Softening, Localization, Regularization, Lip-field

The Lip-field approach is a new regularization method for softening material models. It was presented first in [1] providing one-dimensional simulations for damage and plasticity and was recently extended and implemented for two-dimensional problems [1]. In the Lip-field approach, the mechanical problem is formulated as the minimization of an incremental potential, function of the displacement field and internal variables. The potential itself is not regularized and has essentially the same form as in a local formulation. It does not contain any term depending on the spacial variations of the internal variables (like the Lapalacien) as is the case in typical phase-field approach [3, 4]. In the Lip-field approach, the regularization comes from the addition of a **Lipschitz** constraint on the damage field. In other words, the difference between the damage values at any two points must be less than the distance them, divided by a characteristic length. A discrete version of the Lipschitz constraint in the context of the finite element-method is constructed, defining a convex discrete subspace. Then a resolution scheme is presented, based on an iterative staggered scheme. The displacement field is sought for a given damage field by minimizing the potential with regards to the displacement, leading to classical equilibrium equations. Then at fixed displacement, the damage field is the minimizer of the potential, under the discrete Lipschitz constraint, the latter leading to a convex minimization, with convex constraint, solvable with standard interior point cone programming. In order to drastically reduce the complexity, we detail the construction of bounds of the subdomain where the constraint need to be explicitly unforced. The contribution is concluded by two-dimensional examples demonstrating the capability of the approach.

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Modeling Combined Necking Cracking Phenomena in Thin Metal Structures

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Key Words: *Solid-like shell, XFEM, Failure, Thin-walled structures, Necking, Traction separation law*

Marine structures subjected to different extreme conditions may undergo large inelastic deformation, leading to the formation of highly localized zones of intense straining and, ultimately to the onset of fracture and failure. The experiments performed on thin metal sheets under different loading conditions have shown a competition between necking and cracking phenomena [1]. Furthermore, Woelke et al. [2] showed that the traction separation law that governs the failure process zone after crack initiation, evolves as a function of crack extension because the law is affected by the evolution of necking ahead of the crack tip. Therefore, the relationship between stress state, boundary conditions, and necking need to be thoroughly investigated in order to incorporate necking and cracking initiation and evolution into a physically based objective failure model. This contribution focuses on a continuum modeling approach combined with a discrete modeling approach (XFEM) to simulate the interaction of necking and cracking phenomena. XFEM is incorporated into a geometrically nonlinear discontinuous solid-like shell element [3] to simulate failure in thin-walled structures. Special attention will be given to obtain an objective traction separation law for the cohesive zone modelling, and failure initiation and orientation criteria. The criteria for the requested mesh density come from the curvature of crack and a proper representation of stress and strain field in a cracked region. The required mesh size that can properly capture local effects for accurate calculation of crack initiation after necking and subsequent crack propagation will be demonstrated in this contribution.

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Modelling the anisotropic damage of concrete under tensile loading at the mesoscale

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Key Words: anisotropic damage, concrete, constitutive modelling, ABAQUS, thermodynamics, elastic–brittle material, damage mechanics, tension

The development of an elastic brittle anisotropic damage constitutive model for plain concrete at the mesoscale under tensile loading is presented. At this scale concrete is considered as a three-phase heterogenous material consisting of aggregates, cement mortar and interfacial transition zone (ITZ). In this work the aggregates are considered as elastic undamageable inclusions, while a thermodynamically consistent tensorial damage model is used for the cement mortar in conjunction with a traction separation law for the ITZ. Within the framework of continuum damage mechanics (CDM), the theory of internal variables, the thermodynamics of the irreversible processes, the effective stress and energy equivalence hypotheses are used such that the three-dimensional constitutive equation of the elastic brittle damageable cement mortar is written in the effective (undamaged) configuration.

Within a thermodynamic framework, the damage initiation and evolution mechanism in the elastic range due to Mode I, II and III micro-crack propagation in the ITZ and in the cement mortar under tension is investigated. The different contributions of the second-order damage tensor components to the mesoscopic anisotropic reduction in stiffness of concrete are also demonstrated.

The damage model is implemented into the advanced FEA program (ABAQUS/standard) through a user-defined material subroutine (UMAT). This work shows that the mesoscopic damage is initiated and begins to evolve and the micro-mechanical properties of concrete start to degrade earlier than that observed at the macro level. The performance of the presented phenomenological framework is verified by comparing the numerical predictions with the experimental tests of concrete under monotonic uni-axial tension.

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Molecular dynamics Analysis on the degradation of the crystallinity of a grain boundary under creep loading at elevated temperature.

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Key Words: *Molecular Dynamics, Bicrystal, Creep Damage, Plastic Deformation, Crystallinity of a Grain Boundary,*

Abstract:

Since the drastic decrease in the lifetime of heat-resistant alloys under creep and creep-fatigue loads at elevated temperatures was attributed to the acceleration of intergranular cracking [1], the degradation of the crystallinity around a grain boundary, which causes brittle intergranular cracking under creep loading at elevated temperatures, was analysed by using a molecular dynamics analysis of a bicrystal structure. The local crystallinity was found to be degraded by the accumulation of dislocations and vacancies around the cracked grain boundaries [2]. In this study, the GEAM (Generalized Embedded Atom Method) interatomic potential was optimized for the analyses at elevated temperatures. The potential parameters were optimized to reproduce lattice constant, cohesive energy, elastic constants and melting temperature within the error of 5%. The determined potential explained these physical parameters well. The deformation and fracture behaviour of bicrystal structures were analyzed at 973 K, which is the representative operating temperature of the advanced thermal power plants.

It was found that the stress relaxation appeared even under the application of uniaxial stress of which magnitude was 50% of the yielding stress of the bicrystal structure. This stress relaxation was caused not by growth of dislocations but by the activation of atomic diffusion around the grain boundary. Outdiffusion of component atoms from the grain boundary region was accelerated at elevated temperature. Slight grooving also started to appear in the grain boundary region. The outdiffusion was drastically accelerated when the lattice mismatch between the nearby grains became large. The lattice-mismatch-induced local strain distribution caused the acceleration of atomic diffusion around the grain boundary. The drastic decrease in the density of atoms around the grain boundary degraded the effective strength of the grain boundary, and thus, intergranular cracking was accelerated by the degradation of the crystallinity around the grain boundary. These analytical results agreed well with the experimental results of the accumulation of vacancies and the degradation of the strength of grain boundaries with large lattice mismatch. The local concentration of free energy around the grain boundary was found to be a driving force of the outdiffusion. The local concentration of free energy was attributed to the strain energy caused by the lattice mismatch and mismatch of elastic constant between the jointed grains in the bicrystal structure. The concentration field was explained by using the modified Arrhenius equation where the effective activation energy changed as a strong function of mechanical stress.

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Numerical Prediction of Crack Initiation and Propagation for Spot Welded Joints of Advanced High-strength Steel Sheets

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Key Words: *Spot welding, High-Strength steel, HAZ, Crack Growth, Finite Element Analysis*

It is common to use spot welding when assembling high-strength steel plates for automobiles. Because of the effect of Heat Affected Zone (HAZ) generation where spot welding is applied, there is a problem in the accuracy of predicting the fracture of the spot-welded material [1][2], and the deformation behaviour of the vehicle body cannot be accurately reproduced. In addition, since there are many welding combinations such as steel grades and the difference in plate width and plate thickness, a general evaluation method is difficult to be established. Therefore, the aim of this paper is to develop a crack initiation and propagation prediction method for spot welded steel plates that can be applied to various combinations of steel grades and thicknesses.

Tensile tests were conducted on spot-welded high-strength steel sheets of 590 MPa, 980 MPa and 1180 MPa grades. The fracture strength and fracture strain were obtained and crack initiation and propagation behaviour were observed. In addition, fracture surfaces were observed with a scanning electron microscope, and the location of crack initiation and crack propagation mechanisms were analysed.

Also, micro-tensile tests were performed using micro test pieces collected from the spot-welded steel sheets to clarify mechanical properties around welding zone. Meanwhile, Vickers-hardness around HAZ was measured by nanoindentation tests. Based on above experimental results, we introduced shift factors of stress-strain curve around the spot welded zones and finite element model of spot-welded steel sheets were developed. Then, numerical simulations were carried out and compared with experimental results.

The results show that the fracture strength and fracture strain of spot-welded high-strength steel sheets were quantitatively predicted, and crack initiation and propagation behaviours were also reproduced successfully.

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Numerical prediction of strain-induced crystallization under complex loadings

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Key Words: *Crystallization, Multiaxial loadings, Damage, Multiscale modelling, Infrared thermography.*

As a type of phase transition in natural rubbers, strain-induced crystallization is a phenomenon where amorphous polymer molecules transform to crystallites under the course of extension. Strain-induced crystallites are assumed to play an important role in the self-reinforcement and the crack growth resistance of natural rubbers. In this contribution, strain-induced crystallization of natural rubbers under various loading scenarios is investigated numerically. To this end, a finite element computational framework is constructed on the basis of a recently developed theory for strain-induced crystallization [2]. Its prediction is validated with infrared thermography-based quantitative surface calorimetry measurements under equibiaxial loading condition [1]. Finally, generalization of the computational model in biaxial tension with different biaxiality ratios will be used to analyze the self-reinforcement mechanism in natural rubbers.

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Prediction of Dispersion of Fracture Toughness by Enhanced GTN Model in Ductile-to-Brittle Transition Region

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Key Words: *Stochastic Collocation Method, GTN Model, Cohesive Zone Model, Ductile-To-Brittle Transition Region*

The contribution of this study is to discuss a dispersion of a fracture toughness predicted by the enhanced Gurson-Tvergaard-Needleman model (GTN model) [1, 2, 3, 4] within the ductile-to-brittle transition region. The enhanced GTN model, which has been devised to incorporate a cohesive zone model into a GTN model, is employed to realize the complex fracture behavior owing to the transition from a ductile fracture into a brittle fracture according to the temperature change in metallic materials. The GTN model represents the shrink of the yield surface with increase in void volume fraction due to void nucleation, growth, and coalescence. On the other hand, the cohesive zone model realizes the process of stress release along with the brittle crack propagation after the maximum principal stress reaches local tensile strength. The variation of dispersion of the fracture toughness due to temperatue change is predicted by assessing the uncertainties of both the void nucleation and the local tensile strength in our finite element simulations equipped with the enhanced GTN model. The obtained numerical results are statistically evaluated by stochastic collocation method [5]. In addition, we represent the change of the dispersion of the fracture toughness by introducing dependence of the initial yield stress, hardening behavior and local tensile strength on temperature in the enhanced GTN model. To demonstrate capability of our developed numerical analysis, the cumulative density function of the fracture toughness is compared with that obtained by the experiments at the low-, room- and ductile-to-brittle transition temperatures.

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A coupled immersed boundary-material point method for shock-structure interaction and dynamic fracture

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Key Words: *shock-structure interaction, dynamic fracture, immersed boundary method, material point method, Riemann solver*

Shock-structure interaction is a class of extreme fluid-structure interaction (FSI) problems and always leads to dynamic fracture and fragmentation of solid structures in engineering applications. For its importance in safety and security, this problem has attracted extensive attention in recent decades. And, the development of efficient and powerful algorithms to simulate these phenomena is an active field of research.

Since being first introduced by Peskin[1] in 1970s, the immersed boundary method (IBM) has shown its success in simulating the interaction between fluid and structure with complex boundary geometry. Mittal and Iaccarino[2] classified IBMs into continuous forcing approach and discrete forcing approach based on the way of applying FSI boundary conditions.

Dynamic fracture simulations involve extreme structure deformation and nonlinear material constitutive relation. To avoid the numerical difficulties of distorted grid in Lagrangian method and historical variables recording in Eulerian methods, Harlow[3] proposed the particle-in-cell (PIC) method which discretizes the fluid into Lagrangian particles and computational domain into a uniform Eulerian mesh. Sulsky et al. extended the FLIP PIC method from fluid mechanics to solid mechanics and named this method as material point method (MPM)[4, 5].

The present work combines the concepts of continuous forcing approach and discrete forcing approach, and proposes a novel IBM which can guarantee the boundary velocity conditions strictly at each time step and has no need to keep track of FSI interface anymore. Therefore, the IBM presented here is a promising method for simultaneous simulations of shock-structure interaction and dynamic fracture. And then a method coupling the present IBM with the standard MPM, named CIBMPM, is proposed to simulate the interaction between shock wave and solid structures. The numerical results are in good agreement with several classical shock-structure interaction experiments with fixed or moving obstacle. Finally, the CIBMPM is used to simulate fragmentation driven by detonation and provides a better result than the standard MPM.

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An Explicit Phase-Field Material Point Method for Dynamic Brittle Fracture Problem

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Key Words: *Explicit Phase-Field, Material Point Method, Dynamic Fracture, Stability Analysis*

The phase field method is an effective method to simulate arbitrary crack propagation, branching and convergence. Material Point Method (MPM) combines Eulerian method and Lagrangian method, which has advantages in simulation for large deformation problem. The implicit Phase-Field MPM [1][2] has been studied by many researchers for quasi-static fracture problem. However, few work has been presented to study the application of the explicit Phase field on MPM. Due to the iteration in updating phase field of particles, the implicit Phase-Field MPM has poor simulation efficiency and is inappropriate for dynamic fracture problem. On the contrary, explicit phase field is established by importing the viscous dissipation of phase field evolution. And the phase field can be updated with forward difference scheme which avoids the iteration. In this work, A novel explicit Phase-Field Material Point Method (exPFMPM) is introduced for simulation of dynamic fracture problem in elastic media. Many studies have been done in explicit Phase Field Finite Element Method (FEM) [3][4], but few works study the stability of the time integration of explicit phase field. In this work, the effect of particle position and neighbouring cell interaction on stability of exPFMPM is studied. An explicit critical time step formula is obtained based on the system eigenvalues in one dimension, and is then extended to two and three dimensions. And the critical time step formula can also be used in explicit Phase Field FEM. Several tests are performed to verify the critical time step formula. The effectiveness and validity of the exPFMPM method is assessed through several numerical examples (Three-point bending, Dynamic crack branching, ie) for dynamic fracture in brittle materials.

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An Immersed MMALE Material Point Method for FSI Problems

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Key Words: *material point method, multi-material arbitrary Lagrangian Eulerian method, fluid-structure interaction, immersed boundary*

The simulation of the fluid–solid interaction (FSI) problem is important for both academic studies and engineering applications. However, the numerical approach for simulating the FSI problems is a great challenge owing to the large discrepancy of material properties and inconsistent description of grid motion between the fluid and solid domains. The difficulties will be further increased if there are multiple materials in the fluid region and large deformation and fracture in the solid region.

Material point method (MPM) provides a powerful tool for modeling extreme deformation and fracture in solid, as well as multi-material arbitrary Lagrangian Eulerian method (MMALE) shows great capability to simulate compressible fluid with multiple materials and shock waves. On the basis of an analogous scheme formulation between the above two methods which consists of Lagrangian variables updating and Eulerian remeshing, an monolithic immersed MMALE material point method is proposed in this work to simulate the FSI problems with compressible fluid and solid of arbitrary constitutive models. In the novel method, the fluid-structure interactions are implicit and fluid-structure interfaces are automatically captured, so that the method could dealing especially well with the FSI problems where structure damage is induced under complex fluid load. Several examples in this paper illustrate the behavior of this novel method.

An Improved Efficient Molecular Simulation Method for Graphene

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Key Words: *Molecular Simulation, Dual mesh, Multiple time step, Graphene*

The graphene, as one typical 2D material, has demonstrated its extraordinary mechanical, chemical, electronic and thermal properties. The molecular dynamics (MD) method is a widely used and practical numerical tool for studies on the physical properties of graphene. However, complicated potentials in the graphene system and huge degrees of freedom (DOFs) lead to tremendous computational cost in MD simulation, which limits the applicable spatial and temporal scales. Smoothed molecular dynamic (SMD) method is an efficient molecular simulation method by introducing a set of background mesh and mapping process into molecular dynamics (MD) procedure. A much larger feasible time step can be adopted for the high-frequency modes are suppressed. Inheriting the high efficiency of the original SMD method, we present some improvements for SMD to achieve a proper multiscale mechanical model for graphene simulation in this report.

A dual mesh (DM) scheme is developed according to the lattice structure of graphene, which contains two non-equivalent carbon atoms. Two sets of background mesh are used in DM-SMD and the physical variables of all the atoms in one type will be mapped onto the same mesh, so that the excessive average between different atoms is avoided and the accuracy can be shapely increased. The multiple-time-step scheme is adopted in MD-SMD coupling method. Besides, an adaptive scheme for identifying MD region is developed, where the MD and SMD regions can be automatically alternated during the simulation. The proposed method is validated with several typical examples of single- and multiple-layer graphene and the results demonstrate great accuracy and efficiency.

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Material Point Method for Growth-induced Massive Deformation Analysis of Soft Materials

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Key Words: *Material Point Method, Soft materials, Mass growth, Massive deformation, Volumetric locking*

To analyze the growth-induced massive deformations of incompressible soft materials, a material point method (MPM) with a total-Lagrangian formulation was proposed. In this method, the mechanical behavior coupled growth and large deformation is handled within the framework of the MPM based on the multiplicative decomposition of the deformation gradient. A mixed MPM formulation was developed by supplementing a weak-form equation for hydrostatic pressure to avoid the volumetric locking caused by the incompressibility of soft materials. To deal with the cell crossing noise caused by the massive deformation, the total-Lagrangian formulation was further introduced into the mixed MPM. the B-spline basis functions were implemented to the MPM to achieve a high-order accuracy and satisfy the LBB condition. The efficiency and accuracy of the proposed method were demonstrated by several representative two- and three-dimensional numerical examples, such as the free growth of blocks and constrained growth of rings. Some practical problems, including the bending of star and the strain-driven growth of human skin, were further investigated using the proposed MPM to illustrate its ability and potential for evaluating and analyzing the growth phenomena and behaviors observed in nature and engineering. This work was supported by the NSFC (Nos. 12072062 and 12072061), the LiaoNing Revitalization Talents Program (XLYC1807193), Key Research and Development Project of Liaoning Province (2020JH2/10500003) and Fundamental Research Funds for the Central Universities (DUT20LAB203).

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Modeling and Simulating Method for Dynamic Crack Propagation in Residual Stress Field

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Key Words: Residual Stress, Fracture Analysis, PDS-FEM, Tempered Glass

Residual stress field is a self-equilibrium state of stress in the bulk solid materials induced by inhomogeneous inelastic deformations. The residual stress has a great influence on dynamic crack propagation process. The compressive residual stress prevents crack initiation and growth, while the tensile residual stress leads dynamic fracture resulting in the instantaneous and catastrophic destruction.

The dynamic crack growth is accompanied by the release and redistribution of the residual stress. The interaction between the dynamically growing cracks and the residual stress field is complicated enough for preventing us from building effective models, and thereby this phenomenon is left unsolved in the field of solid continuum mechanics.

In this study, we propose a mathematical model and a numerical analysis method for the dynamic fracture in residual stress field. We formulate the dynamic behavior of solid continuum with residual stress field in the context of Particle Discretization Scheme Finite Element Method (PDS-FEM). This formulation enables the evaluation of release and redistribution of the residual stress due to fracture, and the effect of the elastic wave on crack propagation.

By using the proposed model and method, we perform the simulation for the dynamic crack propagation in chemically tempered glass sheets with different residual stress intensity. Our simulation results successfully demonstrated the crack pattern and the crack propagation speed in each tempered glass sheets. These results show that the proposed model and method can be a general framework to simulate the release and the redistribution of the residual stress in the dynamic fracture process.

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Numerical Simulation of Projectile Penetrating Based on Improved SPH Method

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Key Words: *Smoothed particle hydrodynamics, Penetration, Numerical fracture*

SPH (smoothed particle hydrodynamics) is a gridless Lagrangian technique that is attractive as a possible alternative to the numerical techniques used to analyze large deformation events. In the conventional SPH method, numerical fractures result due to the loss of interactions among particles, which annoys the ability and the accuracy of SPH simulation method. To prevent the numerical fractures, the improved SPH method, which periodically reinitializes (remesh) the particle locations that are being distorted by the serious deformation, and the new particle generation techniques are carried out for the projectile penetration process on aluminum alloy target. Through the numerical simulation, the stress responses of target under different impact velocities are discussed. The relationship between the residual velocity of the projectile and the initial velocity is simulated and analyzed, as well as the failure modes of the aluminum alloy target plate under different impact velocities. The results show that the improved SPH method solves the numerical fracture problem effectively and can describe the physical fracture very well with better accuracy. Meanwhile, the numerical calculation results are in good agreement with the experimental results. The obtained results elucidate the fracture mechanism of target materials under different stress states and provide a theoretical prediction method for experiments, which has certain guiding significance.

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Numerical simulation of splashing water trajectory under engine influence

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Key Words: *Aircraft tyres, Splash water trajectory, Engine flow field, Impact load*

When the aircraft pass through the contaminated runway, its tire splashing may affect the safety of the plane. The side spray of the front landing gear may enter the inlet of the engine and affect the normal operation of the engine. In this paper, the tire splash model under different speed conditions was established by SPH method in LS-DYNA, and the initial shape of tire splash was obtained through simulation. The engine flow field was simulated by CFX, and the velocity information of the engine flow field was obtained. Then the SPH particles in the initial stage of splash water were simplified to droplets and their position, velocity information and engine flow field information are imported into MATLAB. Tire splash trajectories, engine water ingress and impact forces were calculated for different water depths and speeds. Finally, the calculated results are in good agreement with the tire splash test results. The research method can be applied to calculate the splash shape and load of different tire shapes and pollutants, and promote the application of tires with chine configuration, and provide ideas for the morphology and load calculation of the cook-tail water spray.

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The Abnormal Change of Fluid-Solid System Induced by the Confinement with Extreme Small Size

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Key Words: *Nanoconfinement, Water, Machine Learning, Molecular Dynamics*

Fluid-filled porous materials are ubiquitous in nature, such as the shale, soil, bone, plant stem and so on. They also possess wider and wider applications in the modern industry, such as microfluidic channel for cooling, virus detection and so on. Understanding the abnormal change of such fluid-solid system especially with extreme small channel is significant for understanding natural phenomena and applying in industrial engineering. In this work, we focus on the numerical simulation of the water confined in small channel. Firstly, based on the machine learning method, two high-precision water models TIP4P-BG (a conventional four-site water model) and TIP4P-BGT (an advanced model with temperature-dependent parameters) are established. Both the water models exhibit excellent performance with a reasonable balance among the four crucial physical properties. The relevant mean absolute percentage errors are 3.53% and 3.08%, respectively. Subsequently, the controllable deformation of fluid-filled channel through filling with salt water and applying an electric field is examined. With the electric field along the axial direction, the height of CNTs is enlarged by the axial electric force due to the internal ions and polar water molecules. Under an electric field with two mutually orthogonal components, the transverse electric force could further induce the bending deformation of CNTs. Finally, based on the salt water-filled carbon nanotubes, a separation membrane with the adjustable molecular channels by the electric field is proposed. The successive separations and the switch between the high-efficiency and high-purity separation could be achieved only through adjusting the electric field intensity. The reported finding provides a foundation for water-filled small-size channels and provides an insight into the design of nanoscale functional devices. The supports from the National Natural Science Foundation of China (Nos. 11972108, 11672063, 12072061, and 12072062), the LiaoNing Revitalization Talents Program (XLYC1807193), the 111 Project (No.B08014) and Fundamental Research Funds for the Central University are gratefully acknowledged.

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Time-discontinuous Peridynamic Method for Transient Crack Propagation Problems

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Key Words: *crack, peridynamics, stress wave propagation, time-discontinuous formulation, transient problem, contact impact*

A time-discontinuous peridynamic method (TDPD) was developed to accurately simulate the sharp gradient features of the elastic-plastic stress wave propagation and reduce spurious numerical oscillations in transient problems. In this method, the displacement field and the velocity field are interpolated independently using cubic Hermite functions and linear functions in the temporal domain respectively, which are allowed to be discontinuous between the adjacent time steps. The weak form and a new time integration scheme were derived by combining the peridynamic governing equations with the time-discontinuous method. The displacement field is continuous while discontinuous jumps are introduced into the velocity field. The TDPD can effectively characterize discontinuous characteristics of stress and eliminate spurious numerical oscillations that usually appear in the transient solutions obtained by the PD with conventional time integration method for transient problems. Numerical results of many representative problems demonstrated that the TDPD can effectively suppress the spurious numerical oscillations and predict reasonably the crack propagation. The ability of TDPD to accurately predict the initiation and propagation of cracks was also demonstrated through several representative problems involving dynamic fracture. In addition, some 3D contact impact and engineering examples were given, illustrating the broad prospects of TDPD in engineering applications. This work was supported by the NSFC (Nos. 12072062 and 12072061), the LiaoNing Revitalization Talents Program (XLYC1807193), Key Research and Development Project of Liaoning Province (2020JH2/10500003) and Fundamental Research Funds for the Central Universities (DUT20LAB203).

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A variational phase-field model of fracture with frictional sliding

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Key Words: Phase-field models of fracture, Gradient damage models, Frictional sliding

The phase-field model has become a popular computational approach for fracture over the past two decades [1]. One of the strengths is its ability to trace propagating fractures without explicit representation of fracture. While this implicit representation facilitates simulation of complex fractures, it obscures explicit properties such as crack opening displacements or stresses resolved on crack surfaces. For this reason, phase-field models have not been extended to frictional sliding, which requires the normal and the tangential stress components on the sliding surface, until the recent work by Fei and Choo [2]. They proposed to decompose the stress at fracture interface into the frictional and non-penetrating components, and iteratively determine the frictional stress using Coulomb's friction criterion. Though their model is able to resolve stresses at interface properly, the mode of fracture propagation is limited to shear (mode-II). In this study, we propose a variational phase-field model with frictional sliding by considering the plastic strain in the sliding direction and the plastic blocking energy in the strain energy as:

$$\Psi(d,\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^{\mathrm{p}}) = \begin{cases} \dfrac{1}{2}\mathbb{C}(d):\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon} & \text{if open,} \\ \dfrac{1}{2}\mathbb{C}:(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\mathrm{p}}):(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^{\mathrm{p}}) + \dfrac{1}{2}\mathbb{H}(d):\boldsymbol{\varepsilon}^{\mathrm{p}}:\boldsymbol{\varepsilon}^{\mathrm{p}} & \text{if in-contact,} \end{cases}$$

where $\mathbb{C}$ is the tangential stiffness tensor, d is the damage, $\boldsymbol{\varepsilon}$ is the strain, $\boldsymbol{\varepsilon}^{\mathrm{p}}$ is the plastic (sliding) deformation, and $\mathbb{H}$ denotes the stiffness degradation by the sliding. We find $\mathbb{H}(d)$ so that it ensures the continuities of the stress and the thermodynamic forces at the open–contact transition. The plastic deformation is computed using Coulomb's criterion as the yield function with an associated flow rule. We demonstrate through examples that our model is capable of capturing the frictional sliding behaviors and unrestricted modes of fracture propagation.

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Adaptive Phase Field Modeling of Brittle Fracture Using the Scaled Boundary Finite Element Method in 3D

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Key Words: Phase field, Hybrid formulation, Staggered scheme, Brittle fracture, Scaled boundary finite element method (SBFEM)

During the last decade, phase field modeling for fracture has attracted much interest in the engineering world because of its impressive capability to handle arbitrarily complicated fracture phenomena also in three dimensions. However, to accurately capture the crack in a diffusive manner, a small positive length scale parameter l_c is required to characterize the width of the regularized crack. The requirement that the element size should be less than half of the length scale renders the method computationally expensive [2]. In this work, an adaptive phase field simulation of fracture in 3D is proposed using a combination of a phase field formulation and the scaled boundary finite element method (SBFEM). Image-based modeling is used to represent the 3D geometries. Taking the 3D image array as an input, the model is automatically decomposed into an octree mesh consisting of regular hexahedrons. The octree mesh is subjected to the 2:1 rule, which determines the size ratio between two adjacent hexahedrons. Hence, the computational effort is reduced by only solving for the unique element configurations.

The SBFEM is used to analyze the balanced, automatically generated mesh. It is a semi-analytical method that facilitates the construction of polyhedral elements where only the faces of the domain are discretized [1]. To achieve accuracy of both the phase field and the elastic analysis, an error indicator based on the SBFEM solution is used to refine the mesh. The staggered solution scheme outlined by Miehe et al. [2] is used to solve for brittle fracture in solids. The hybrid phase field model is adopted, where the phase field variable is assumed to be governed only by the tensile elastic energy, which leads to a linear stress–strain relation [3]. Several benchmark examples are extended to 3D and verified to illustrate the proposed approach.

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An Efficient Phase Field Model for Fatigue Fracture

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Key Words: phase field, fatigue fracture, effcient

The core idea of the phase field model is to represent a discrete, discontinuous phenomenon with a smooth function. For fracture mechanics an additional field variable is introduced to describe the crack. The biggest advantage of the phase field fracture model is its unified framework of the entire crack evolution behavior, including nucleation, propagation, branching, kinking. These phenomena can be covered by one single model. The phase field fracture has been successfully applied to a quasi-statics case. However, there is still a lack of studies on how to efficiently simulate the fatigue fracture phenomenon. In this work, we propose an efficient phase field schemata for cyclic fatigue simulation.

We extend the model from Kuhn and Müller [1] with an additional potential energy term, which provides the necessary driving force for the fatigue fracture evolution. This additional potential is related to the newly introduced damage parameter, representing the damage caused by cyclic fatigue. The additional potential energy is coupled with fatigue parameters from the S-N diagram, which allows the model to generally and elegantly integrate all the influence from the environment to the fatigue propagation behavior. The evolution of the crack field is derived from the total energy with the help of variational principal. The model is consistent with the empirical fatigue propagation property, including the Paris' law and mean stress effect. The model is also robust under complex load simulations.

Traditionally, the fatigue simulation suffers from its huge computational effort since the fatigue crack will only occur after a large number of loading cycles. The cycle number increment influences the computing time of the fatigue simulation and impacts the crack patterns. Thus, the cycle number increment choice is a critical point in the phase field fatigue simulation. We introduce an adaptive cycle increment algorithm, where the cycle number increment is associated with the fatigue damage increment. Our algorithm provides a moderate computing time without losing accuracy compared to the classical computing strategies. Our method is also suitable for parallel computing.

The model has been applied to three-dimensional problems with the real material property. The fatigue life obtained from the phase field model can be verified by experimental and analytical findings.

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Fully coupled damage evolution of moisture effects in polymer matrixed composites

The understanding of water penetration, diffusion, and swelling-related strength degradation is critical for assessing the durability of polymer-based composite materials exposed to marine environment. When moisture intrusion and various external loads are concurrently applied to polymer matrix materials, the multi-physical diffusion process, and the correlation with the complex cracking phenomenon is far from been discovered. To approach this uncertainty, we explored fully coupled moisture diffusion, stress redistribution, and damage evolution of composites for revealing complex failure patterns and rules. In our recent work, a thermodynamically consistent moisture diffusion model is established to couple the moisture diffusion and viscoelastic response of the multiphase material. A two-constituent phase-field fracture model is developed to describe the hygroscopic swelling in the matrix and interfacial decohesion within a concise and universal continuum mechanics framework. We also propose a crack filter theory to characterize the fluctuation of moisture flux along with the evolution of regularized discontinuities. A static strength evaluation index is devised to calibrate the moisture resistance of fiber/polymer composites. Based on the strongly coupled scheme, the distinct damage profiles of dry and immersed composites were captured in line with experimental observations. For the first time, interactions of moisture diffusion with the complex cracking in composites are elucidated through simulations, thus providing new insights into the coupled damage mechanism of polymer composites and facilitating microstructure design to enhance its performance in ocean environments.

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Influence of material properties and fracture properties on crack nucleation and growth in thin films

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Key Words: fracture,desiccation, phase-field, heterogeneous materials, random fields

The fracture of thin films bonded to compliant substrates presents a number of challenges to model-based simulations. Typically, the films are assumed to be subjected to a bi-axial state of stress that arises due to a mismatch in material properties with the underlying substrate. The film can quickly become ovestressed, giving rise to pervasive crack nucleation and growth. Our current work looks to build on recent efforts studying the influence of bulk and fracture properties on crack patterns in these systems using a cohesive-based phase-field model of fracture [1]. In particular, we examine results obtained using an adaptation of a recently developed phase-field model that employs a stress envelope to control crack nucleation [2]. We examine the sensitivity of the simulated crack patterns to variations in model parameters responsible for both nucleation and growth. Results are compared to our previous studies in which crack nucleation was governed entirely by energetics.

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Micromorphic phase-field fracture model: Performance assessment and benchmarking

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Key Words: Phase-field, micromorphic, fracture irreversibility, variational inequality , AT1, AT2

The phase-field fracture model has emerged as a promising alternative to discrete fracture models (e.g., cohesive zone and extended finite element models) owing to its straightforward handling of of complex fracture topologies (crack branching, kinking and merging) and circumventing the need for remeshing techniques. In this model, the fracture is represented by the phase-field, which, along with the displacement field are the primary nodal unknowns. The enforcement of the fracture irreversibility constraint in conjunction with higher regularity requirements on the phase-field (H1 space) results in a 'global' variational inequality problem. In this contribution, a micromorphic phase-field fracture model [1] is proposed. In this model, the micromorphic variable regularizes the fracture problem, while the phase-field is transformed into a local quantity. As a consequence of the latter, the enforcement of the fracture irreversibility constraint is relatively easier to treat in a computational framework. The energy functional for the micromorphic phase-field fracture model is obtained upon replacing the phase-field in the gradient term with a micromorphic variable, followed by penalizing the difference between the phase-field and the micromorphic variable. Both AT1 and AT2 brittle fracture models have been addressed in this contribution. Unlike the history variable approach, the micromorphic AT1 variant does not require a fictitious initial energy to represent the intact material state. Adopting benchmark problems, a performance assessment is carried out whereby the iterations required for convergence, the choice of the penalty parameter, and possible convexification measures (time-lagging, extrapolation) are addressed.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Microstructure sensitive fatigue crack growth in anisotropic polycrystals

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Key Words: Fatigue crack growth, Multiphase-field method, Polycrystals, Grain boundary strength, Material anisotropy

Accurately quantifying the resistance of mechanical component to fatigue crack growth is an essential part of predicting component lifetimes. For a polycrystalline material where each crystal has a different orientation, mechanical characteristics (e.g. Young's modulus, Poisson's ratio, fracture toughness), and associated anisotropies, fatigue crack growth prediction becomes extremely complicated and challenging. To this end, a multiphase-field model for simulating fatigue crack growth in brittle anisotropic polycrystal is proposed which utilises recently introduced [1] fracture toughness reduction as the measure to account for rate- or cycle-dependent crack growth phenomena. The formulation of phase-dependent fatigue strength, which accounts for differing fatigue properties of different crystals, is a significant and innovative component of this research. The multiphase-field formulation also allows to mimic different grain boundary energy (e.g. weaker or stronger grain boundary) of the polycrstalline material [2]. The proposed model is capable of simulating complex crack trajectories under fatigue loading in the complete parameter space, including inter- and transgranular fracturing, where distinct grains have different fatigue properties and preferred planes for crack formation based on fracture toughness anisotropy. Several two-dimensional benchmark problems with multiple cracks are addressed to showcase the capabilities of the proposed model for fatigue crack growth.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Parallel finite element solvers for phase-field modeling of fracture

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Key Words: Parallel computing, FE method, Phase-field models, Fracture mechanics, Preconditioning

Phase-field models (PFMs) are widely used to model fracture in solids. Similar to continuum damage mechanics models, material degradation is described via a scalar-valued phase/damage field ranging from zero (sound material) to unity (fully broken material) and submitted to irreversibly conditions. Damage evolution is modeled by solving a Helmholtz-like damage diffusion equation. The final boundary value problem involves finding a vector-valued displacement field and a scalar-valued damage field that fulfills the non-linearly coupled momentum balance (equilibrium) and damage diffusion equations. Resolution strategies involve either a staggered or a monolithic approach to solving the final boundary value problem. In this work, attention is focused on solvers for the "hybrid" PFM by [1], with the primary objective of developing effective finite element (FE) implementations and to perform large-scale fracture mechanics simulations. Indeed, very refined meshes are needed for solving PFMs in the FE framework for practical problems of interest. Large non-linear systems of coupled equations have to be solved, which makes using these models in large-scale applications a tiresome task due to the high computational workload. Domain decomposition approaches can be used to subdue these issues and considerably decrease computational workload. The computational domain is partitioned into thousands of sub-domains, and the FE linear systems concerning the PFM equations are then concurrently assembled and eventually solved using parallel Krylov subspace methods. Within this contribution, we implement and discuss two ways of setting up domain decomposition parallelism for a hybrid PFM [2] under the distributed computing framework. Particularly, a monolithic FE strategy is compared to a staggered FE strategy. These two methods lead to different matrix sparsities; as such, to yield a fast and robust parallel solver, different preconditioning/parallelization strategies must be applied. Besides presenting the two distinct ways of setting up parallelization for the considered PFM, this article presents a detailed comparison of the performance, scalability, and efficiency of the two methods at massively parallel scales. Overall, this allows for rapid solving non-trivial fracture mechanics problems with millions of unknowns [2].

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Phase-field Modeling of Fracture in Materials with Anisotropic Fracture Energy

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Key Words: Brittle Fracture, Phase-field Modeling, Fracture Anisotropy, Stochastic Fracture Modeling

A large class of solar cell wafers, an integral component of the renewable energy industry, are made of silicon crystal that falls under cubic symmetric class of anisotropic materials. Such a material exhibits, along certain planes, a complicated four-fold symmetry in its elastic parameters as well as in its fracture toughness. Large difference in the amount of energy required for crack propagation along two salient crystallographic orientations gives rise to strong and weak directions, thus leading to strong anisotropy. Additionally, due to cubic symmetry, the two weak directions along which the crack tends to kink are symmetrically located, thus leading to zigzag or saw-tooth crack patterns.

In this work, we follow the well-established phase-field approach for fracture to study cracking in silicon. In particular, we build upon and extend the fourth-order phase-field approximation introduced in [1] containing the second gradient of the phase-field variable in its regularized energy functional in addition to the usual first gradient. A thorough analytical and numerical analysis of the resulting formulation is presented. Furthermore, lack of convexity in the minimization of the coupled phase-field and elastic energy potentials in the isotropic setting gets more severe in the cubic symmetric case given that its fracture toughness, a component of the phase-field energy functional, alone is non-convex. To address this, we transition from a deterministic to a stochastic setting by introducing perturbations in the form of a random field in the anisotropic phase-field energy functional to capture solution non-uniqueness [2]. Such a stochastic phase-field model describes multiple crack paths and their probabilities. The additional insight into the solution behavior, however, requires a larger computational effort. Lastly, results from an experimental campaign undertaken to understand anisotropic fracture in silicon and to calibrate model parameters are discussed. The outcome of this work is hence a well-assessed stochastic phase-field anisotropic module that can be employed to investigate four-fold symmetric fracture anisotropy for complex applications.

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Predicting Fracture in Human Bones using Phase Field Models and the Finite Cell Method

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Key Words: Phase-field fracture, Humerus Fracture, Finite Cell Method

Fracture of the proximal humerus as a result of a fall on an outstretched arm is a common injury among the elderly population. While numerical simulation of bone fracture is a challenging task due to the complex and heterogeneous structure of bone, it is important to advance our understanding of this frequent injury. In this contribution, we present a numerical framework for the simulation of fracture in human bones which is based on a combination of a phase-field model for brittle fracture with the Finite Cell Method (FCM) and adaptive refinement. As presented in [4, 3], integration of the FCM [2] as an embedded domain approach enables the efficient simulation of complex geometries without the need of generating boundary conforming meshes. Multi-level *hp*-refinement allows for a locally refined mesh which dynamically adapts to the crack path. In order to capture fracture in human long bones, the phase-field model was adapted to account for a spatially varying critical energy release rate following [5].

The validity of the phase-field model is discussed based on experimental data of three humeri which were fractured at the anatomical neck [1]. The qualitative comparison of fracture patterns shows very good agreement of computed crack paths with experimental results. Digital Image Correlation (DIC) measured strains as well as experimental failure loads are compared against the numerical computations. The results demonstrate the potential of the proposed framework to simulate fracture in human humeri, and motivate us to attempt a generalization of the model to vertebrae, which will be reported on as well.

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Variationally consistent crack phase-field formulation for ductile fracture

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Key Words: Crack phase-field formulation, Ductile fracture, Damage variable, Flow rule, Evolution law

This study presents a variationally consistent formulation for crack phase-field (PF) modeling of ductile fracture. First, we review the existing models [1, 2, 3], in which emphases are placed on the plastic driving force [1, 3] and degrading fracture toughness [2, 3] that enable PF models to represent the damage evolution in elastoplastic materials. Our attention is also focused on the use of either effective or nominal quantities in the yield function [4] as a new perspective in PF modeling.

Based on these discussions, the formulation of the proposed model is readily made. The constitutive work density consists of stored and dissipated components, in which damage variables are separately introduced for elasticity and plasticity in order to derive variationally consistent evolution laws for plasticity and damage as the stationary conditions of the supremum problem of the dissipative potential related to the constitutive work density. Since such a variational structure of evolution laws has been overlooked or not considered in previous studies, the relevant consideration would provide a new perspective for the crack phase-field community. After the governing equations are derived from the optimization problem within the continuum thermodynamics framework, numerical examples are presented to demonstrate the characteristic feature of the proposed model.

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Calibration of Material Model for Sheet Metals Using Digital Image Correlation and Bayesian Data Assimilation

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Key Words: *Data assimilation, Material modeling, Finite Element Method*

Application of aluminum alloy sheets to automotive components is effective in reducing weight of automotives. However, formability of aluminum alloy sheets is lower than that of steel sheets. To compensate for this disadvantage of formability, it is effective to improve forming techniques of aluminum alloy sheets by understanding the forming limit of aluminum alloy sheets using finite element-based sheet metal forming simulation. In order to improve the accuracy of sheet metal forming simulation, it is necessary to calibrate a yield function and its parameters (i.e., material model) that accurately describes elastoplastic deformation behavior of aluminum alloy sheets. So far, a combination of digital image correlation (DIC) with finite element model updating[1] was proposed as a promissing method to calibrate the material model with high accuracy. However, to the our best knowledge, no material modeling method that can evaluate uncertainty of experimental data has been reported. Therefore, the purpose of this study is to develop a new material modeling method using the data assimilation theory based on Bayesian inference[2] that can evaluate the uncertainties of both experimental and simulation data. In this talk, we present the calibration results of Yld2000-2d yield function[3] using the computationally effcient data assimilation method named as DMC-BO method[4] and a full-field strain measurement by DIC method for a 5000 series aluminum alloy sheet.

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Crystal Plasticity Modeling of Deformation Behavior of a ZX10 Magnesium Alloy Sheet under Various Strain Paths

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Key Words: *ZX10 Magnesium alloy sheet, Crystal Plasticity Modeling, Work Hardening, Twinning, Detwinning*

Magnesium (Mg) alloy sheets are expected to be used as light-weight materials for structural components because of their low density and high specific strength. However, their press formability at room temperature is poor due to the strong crystal anisotropy of the hexagonal structure and the strong basal texture especially observed in AZ series rolled Mg alloy sheets. Recently, ZX series Mg alloy sheets have been developed that weaken the basal texture, thus improving press formability at room temperature [1].

The plastic deformation behavior of a rolled Mg-1.5mass%Zn-0.1mass%Ca (ZX10Mg) alloy sheet was examined in our previous study [2]. It was shown that the in-plane anisotropy of the stress-strain curve was more pronounced under tension than that under compression. Moreover, the tension-compression asymmetry was more pronounced in the rolling direction than that in the transverse direction. In the present study, a crystal plasticity finite-element method was used to study the mechanism of the abovementioned plastic deformation behavior.

A crystal plasticity finite-element method program developed by the authors [3] was used in this study. The material parameters were determined to obtain reasonable fits in the stress-strain curves under tension and compression in the rolling direction. The simulation results were compared with the experimental results of the stress-strain curves under tension, compression, and reverse loading in different directions, and they were qualitatively in good agreements with the experimental results, verifying the model. The simulation results showed that twinning was active not only under compression in the rolling and transverse directions but also under tension in the transverse direction. It was presumed that the difference in twinning activity under tension between the rolling and transverse directions resulted in the abovementioned in-plane anisotropy and the tension-compression asymmetry. In the presentation, results of reverse loading tests will also be discussed.

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Material Model Calibration using 3D-DIC Measurement and Bayesian Data Assimilation

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Key Words: *Data assimilation, Inverse material modelling, Digital image correlation*

Accurate prediction of material deformation behaviors using finite element simulation is important in various industrial fields. In order to improve the predictive accuracy of the finite element simulation, material models including a strain hardening model, a yield function, and their parameters have to be calibrated based on experimental data. In particular, the calibration of material model based on three-dimensional (3D) observation of material deformation behavior is required. For decades, various methodologies for the inverse material modelling using full-field measurements such as digital image correlation (DIC) have been developed [1, 2]. To perform the inverse material modelling, the authors propose to use Bayesian data assimilation (DA) that enables the estimation of unknown parameters and unobservable states of materials by integrating experimental data with the finite element simulation based on the Bayesian inference framework [3]. Although uncertainty quantification in the conventional inverse material modelling remains a challenging issue, DA allows us to evaluate the uncertainty of the identified material model by evaluating covariance of probability density functions of experimental and simulation results. In this study, we propose a new methodology for the inverse material modelling using the ensemble-based four-dimensional variational method (En4DVar) [4, 5] and the full-field 3D-DIC measurement which is one of the most versatile and easiest methods to obtain heterogeneous displacement- and strain-fields over the entire surface of material. By integrating the experimental data obtained by the full-field 3D-DIC measurement to the finite element simulation using En4DVar, it is expected that the material model can be more accurately calibrated. We validate the proposed inverse modelling method by applying it to the estimation of strain hardening parameters and the anisotropy parameters of yield functions (e.g., the Hill and Yld2000-2d yield functions) based on the 3D-DIC measurement of an aluminum alloy specimen subjected to the uniaxial tensile test. In this talk, we will present the result of inverse material modelling using the proposed method.

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Modeling Ductile Response of Anchored Connections Using an Extended Gurson Model

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Key Words: *9 Fracture, Gurson model, shear loading, low triaxiality*

Anchored connections in downhole operations in the Oil & Gas industry are formed by the indentation of tools' setting teeth on the internal surface of deep-well casings. These connections are expected to support loads that are in the longitudinal casing direction, loads include the anchored tools self-weight as well as forces imposed by connected equipment. The loads are supported by the anchored connection shear strength. The scale of the setting teeth is in the range of 1 millimeter, which implies that failure zone around them is in the sub-millimeter scale. Motivated by the non-proportional localized loading on the failure zone through the thickness of the steel casing, we propose the calculation of the strength of this connection using a shear-extended Gurson model.

The successful use of the shear-extended Gurson model is contingent on the model calibration to represent the material response. Therefore, a suite experimental tests were performed to characterize the material failure in different multi-axial loading regimes. The experimental testing results were used to inform the model calibration. The calibrated model is used to assess the anchored connection strength, a two-dimensional plane strain idealization is used. First, the formation of the anchored connection is represented by the indentation of the setting teeth into the casing substrate. This stage captures the localized deformation in the casing surface. Then, a shear loading is applied on the teeth to resemble the applied loads. The dependence of the connection's shear strength on the indentation depth is investigated for an increasing number of setting teeth. The modeling leads to novel insights on the response of the shear-extended Gurson model under combined multi-axial loads. In addition, it leads to the establishment of general trends in the relationship between shear strength and indentation force.

A Multi-Scale Probabilistic Model for Progressive Failure Assessment on Woven Composite Laminates

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Key Words: *Woven composite, Multi-scale, Progressive failure assessment, probabilistic model*

Woven composites have been increasingly applied in aerospace, military and transportation due to their excellent specific stiffness, specific strength, impact resistance and fracture toughness[1]. Reliable evaluation on multi-scale mechanical response and failure process of woven composite structures with the aid of numerical tools remains a challenge and hot issue owing to their complex woven fabric geometry. This paper proposed a multi-scale probabilistic model for progressive failure assessment on woven composite laminates considering the stochastic nature of constituent material properties and random distribution of fibers. Three-scale finite element models with randomly distributed material properties are established to study the mechanical response of woven composites, including microscopic representative volume element (RVE) model of yarn, mesoscopic RVE model of woven composite lamina and macroscopic model of notched woven laminates. Multi-scale failure criteria for woven composites are developed to account for physical failure modes at fine scale and phenomenological failure law at coarse scale. Integrating Monte-Carlo method with progressive failure assessment model, repeated simulations at three scales are performed to obtain the probabilistic distribution of mechanical properties and progressive failure process of woven composites. Good agreement between numerical results and experiments has been achieved.

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Efficient computational Multiscale Method for Polymer solids and Structures under Large number of Cycles

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Key Words: Laplace-Carson inversion, high cycle simulation, periodic basis, polymer structures

In this work, a computational method is proposed for viscoelastic (VE) and viscoelastic-viscoplastic (VE-VP) polymer solids and structures subjected to large numbers of loading cycles. The proposed method uses the Laplace-Carson Transform (LCT), extended for periodic response.

For linear VE materials, the methodology is based on the decomposition of the VE problem into transient and periodic sub-problems invoking the superposition principal. Each one is solved independently in Laplace-Carson domain. Then the transient response in time is recovered by LCT inversion using Schapery's collocation method. For the periodic part, sinusoidal functions decomposition is formulated, and the Newton-Gauss algorithm is employed for the numerical inversion. First, the accuracy of the proposed method is assessed on some known time functions. Next, the procedure is tested for VE structural problems (10k cycles, 2D structures, different boundary conditions) and the results are compared to those of reference solutions computed directly in the time domain. The comparison in local scale (displacement, strain and stress at various points) and macro scale (global energy indicator) shows excellent accuracies. The speedup factor (32 for 10k cycles) increases significantly with the number of cycles.

The proposed method has been extended to thermoplastic polymer solids and structures exhibiting coupled VE-VP material response. A multiscale approach in space and time was developed, taking into account a heterogeneous microstructure (VE matrix, VE-VP weak spots and process-induced porosity) and two time scales: macroscopic (at the end of each cycle) and microscopic (within each cycle). Numerical results showing the accuracy and efficiency of the method on structural problems are presented. This opens the door for an efficient multiscale modeling and prediction of high cycle fatigue.

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Failure analysis of composite materials via micromechanics modelling and deep neural networks

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Key Words: *CFRP, micromechanics analysis, deep neural networks, failure criteria*

Carbon Fibre Reinforced Polymer (CFRP) composites are currently being utilised in many engineering applications due to their excellent design flexibility and high specific strength and stiffness. However, the failure of composites is difficult to predict due to the complex coupling effects of different damage modes under combined stress states. Failure criteria play a vital role in the design of composite structures. The lack of comprehensive experimental data for the validation of computational failure models, especially for composite structures subjected to multiaxial loadings, has led to highly conservative designs.

Numerical modelling is widely used in industry to accelerate composite design and aid failure prediction, using a suite of computational tools including the finite element method, the phase field approach, discrete element method, or peridynamics. Currently, micromechanics-based 3D Representative Volume Elements (RVEs) are widely used to analyse the microscale failure mechanisms of composite materials which lead to macroscale (structural) failure. In this paper, high-fidelity finite element-based 3D RVE models were developed to analyse the failure mechanisms of IM7/8552 CFRP unidirectional (UD) composites subjected to biaxial loading conditions via periodic boundary conditions. The Drucker-Prager plastic damage constitutive model, and cohesive zone model, were utilised to simulate the mechanical response of the matrix and fibre-matrix interface respectively. Fibres were assumed to be transversely isotropic, elastic and brittle, where fibre failure was predicted by the maximum principal stress criterion. After validation of the RVE models with experimental tests under biaxial loading conditions, numerical simulations of other biaxial cases were conducted. Due to the transverse isotropy of the cross section of UD lamina, nine out of fifteen loading stress combinations were selected. For the generation of failure points, defining a failure envelope, an average of ten loading cases were considered for each selected biaxial stress combination. In order to generate enough data from the obtained numerical results, probabilistic failure distributions were attributed to the data points. Normal and Weibull distributions were used to describe the scattering of biaxial data with failure probabilities deduced from off-axial experiments and the mean failure surface determined using a univariate spline function. Because of the limitation of available experimental data, obtained failure envelopes were assumed to be self-similar which meant the failure envelope contracted or expanded with different failure probabilities and shared the same scattering factors with the ones from the experiments. A database, containing half a million samples was collected, and each sample had six stress components as input and provided a probabilistic failure output. A deep neural network with four hidden layers was used to construct the failure criterion for the lamina. The number of neurons in each layer was 128 after parametric study. Good agreement between the true values and predicted values was achieved.

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Implementation of R-curves for trans-laminar fracture of carbon/epoxy laminates using Abaqus Virtual Crack Closure Technique

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Key Words: *fracture, R-curve, FEA, VCCT*

Full-scale structures with notches are sometimes stronger than expected on the basis of Linear Elastic Fracture Mechanics because of the existence of R-curves. An R-curve describes an increase in fracture energy with increasing notch length, which is important for the prediction of notched failure of composite structures. R-curves can be implemented in different Finite Element (FE) modelling schemes such as Cohesive Zone Models [1], High-fidelity Finite Element Models [2] and Continuum Damage Mechanics Models [3]. It is also desirable to implement R-curves using a simple FE modelling method to reduce computational costs when modelling large composite structures. One popular method for modelling cracks is the Virtual Crack Closure Technique (VCCT) based on linear elastic fracture mechanics. VCCT for Abaqus [4] provides extensive fracture mechanics capabilities and can be used as a predictive tool to better analyse the crack propagation behaviour in composite structures. The current study aims to take account of R-curves for trans-laminar fracture of carbon/epoxy laminates using Abaqus VCCT with its nodal energy rate option. This enables the specification of a list of critical strain energy release rates to a set of nodes along the crack surface, effectively implementing an R-curve. The linear R-curves implemented in this study was initially measured by Xu, et al. [5] and extrapolated where data is not available. The Abaqus VCCT predicted load-displacement response will be verified by experiments.

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Inspection Interval Optimization of Aircraft Composite Structure using Finite Element Analysis

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Key Words: *Reliability, Inspection Interval, Optimize, Composite, Finite Element Analysis, Delamination*

In recent years, advanced fiber-reinforced composites have been increasingly applied in aviation and aerospace instead of conventional metallic materials due to their superior properties such as high strength, stiffness, and low weight. Particular attention must be paid to model the delamination initiation and propagation to ensure the composite structures do not fail prematurely. The most important feature for implementing composite materials in aviation is their behavior on dynamic loads and resistance to fatigue. However, there is a lack of numerical procedures to accurately predict the delamination growth in complex composite structures under fatigue loading. Therefore, it is essential to find the response and behavior of aircraft composite structures under fatigue loading. In this study, the progressive damage modeling-based approach (Cohesive zone approach) included in ABAQUS is adopted in conjunction with the Paris law to analyze the delamination in composite aircraft structure under the operating load spectrum fatigue loading. FEA modeling is verified through comparison with experimental specimen data [1], and the verified FEA model is applied to the composite aircraft tail wing structure. In this case, a Monte Carlo simulation is performed by building a response surface model considering the uncertainty of the parameters. Through this process, the risk according to each flight time can be quantitatively evaluated, and the inspection interval is optimized by selecting the combination with the lowest number of repeated inspections within the conditions that meet the permitted risk criteria.

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Mesh independent modelling of tensile failure in composite laminates using mixed-time integration in explicit analysis

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Key Words: *Cohesive zone modelling, Finite element analysis, Composites*

Discrete crack modelling involves representation of cracks in a material as geometric discontinuities. Within a finite element framework, mesh independent crack modelling is performed such that crack propagation is not restricted to element boundaries and can propagate across a mesh. In composite laminates, matrix cracks are usually the first to appear and drive delamination due to stress concentration. Although delamination between plies is restricted to element boundaries in a mesoscale model, transverse matrix cracks in non-fibre aligned meshes are not and thus require mesh independent modelling. A set of non-linear events following matrix crack onset and delamination growth result in the final failure of a laminate along with or without fibre failure. Explicit time integration is preferred to model this nonlinearity numerically and the challenges in modelling are (i) reduction in the stable time increment of an analysis following element splitting and the corresponding increase in computational cost and (ii) challenges in remapping of integration domains and initiation of cohesive segments. To solve the first problem, a mixed time integration or subcycling [1] is introduced adaptively following element splitting. The second problem is solved by initiating cohesive segments between the newly initiated elements with minimal disturbance to the surrounding stress state by nodal force balance. Application of mixed-time integration to crack modelling requires extensive analysis and this work is focussed on the challenges in the implementation, the effects of assumptions involved in subcycling and the computational benefits. Suitable numerical examples are demonstrated by modelling tensile failure in composite laminates. Linear solid elements are used in unstructured meshes where the crack geometry does not align with the initial mesh. Tensile failure of an angle-ply laminate and a quasi-isotropic laminate with an open hole is modelled. Crack initiation is performed adaptively along with mixed time integration. Good correlation with experimental results in terms of failure patterns and failure stress is obtained. Following this, the challenging case of tensile failure of a laminate with an embedded wrinkle is also modelled using the introduced framework. The analysis is numerically stable with 240 matrix cracks and 23 delamination planes successfully modelled to predict a very similar failure stress to experimental results [2].

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Modeling Fatigue Failure in Soft Fibrous Tissue using a Visco-Hyperelastic Model with Discontinuous Damage

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Key Words: *Fatigue Life, Composite Biomaterials, Constitutive Modeling, Cyclic Creep*

Introduction. Soft connective tissue is a fibrous composite that is susceptible to injury from single high-magnitude static loads and repetitive low-magnitude fatigue loads. While many constitutive formulations have been developed to model static failure in soft tissue, a modeling framework has not been established for fatigue failure. The identification of a constitutive framework that can describe and predict soft tissue fatigue failure could help explain this poorly understood failure phenomena and advance the prevention and treatment of fatigue injuries [1]. Here we determined the feasibility of using a visco-hyperelastic damage framework to simulate high cycle fatigue failure in soft fibrous tissue.

Methods. Cyclic creep data from six uniaxial tensile fatigue experiments of human meniscus was used to calibrate the specimen-specific material parameters for a visco-hyperelastic damage model with discontinuous damage (strain energy-based failure criterion) subjected to force-control loading. The optimization of the calibrated material parameters was performed in a custom MATLAB code that simulated a single volumetric element subjected to force-controlled loading. The quality of model fit was quantified using normalized root mean square error. The sensitivity of the model simulations to changes in material parameter values was evaluated, and a validation study was performed by evaluating the model's ability to simulate the stress-strain curve of monotonic uniaxial tensile experiments (static failure).

Results. The model was able to successfully simulate all stages of cyclic creep, including steady-state creep and the rapid progression to tissue rupture for experiments that failed between 150 to 400,000 cycles (NRMSE = 2.4 ± 2.6%). Mathematically, damage propagated under constant cyclic stress due to time-dependent viscoelastic increases in tensile stretch that in turn increased strain energy. Our results implicate viscoelasticity as a fundamental regulator of fatigue failure in soft tissue, where our sensitivity study found that tissue with slow relaxation times is more resistant to fatigue injury. In a validation study, the visco-hyperelastic damage model was able to simulate characteristic stress-strain curves of pull to failure experiments (static failure) when using material parameters curve fit to the fatigue experiments.

Conclusion. For the first time, we've shown that a visco-hyperelastic discontinuous damage framework can model cyclic creep and fatigue failure in soft fibrous tissue. A clear benefit of this approach is that constitutive equations for discontinuous damage and viscoelasticity are well established and are available in commercial and open source finite element solvers [2]. Importantly, our results demonstrate that this modeling framework may enable the reliable prediction of both fatigue and static failures from a single constitutive formulation.

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Numerical Investigation into the Failure Mechanisms of Z-pinned Curved Composite Laminates under Four-point Bending

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Key Words: *Z-pin, Delamination, Finite Element Analysis, Cohesive Element*

Z-pinning entails inserting small rods through the thickness of fibre-reinforced polymer composites, and it has been proved to be very effective on mitigating interlaminar disbond (delamination) for composites. Almost all research on the mechanical applications of Z-pins focuses on delamination growth in flat panels [1], while delamination could also be a dominant failure mode in a curved laminate structure when subjected to a bending moment. Ju et al. [2] experimentally demonstrated that it is feasible to increase the curved-beam bending strength by inserting grooved stainless-steel Z-pins in the curved area. In the current work, further experiments to verify whether carbon-fibre composite Z-pins also show this enhancement effect when inserted in curve laminates are being undertaken. Furthermore, computational simulation is required to have a comprehensive understanding on the failure mechanisms of Z-pinned curved laminates subjected to four-point bending.

A meso-scale Abaqus/Explicit® 3D Z-pinned curved laminate model was built in this study. The model was created with a versatile mesh generation code, which was written by combining Python and MATLAB®. The user is able to control almost all the input parameters, such as pin number and spacing, stacking sequence, fibre orientation, roller diameter and position, material properties and interface definitions, etc. An eye-shape resin-rich zone is modelled around each pin. Cohesive elements were inserted between different-angle plies to simulate delamination. Node-to-surface tie constraints were defined between interlaminar cohesive layers and their adjacent plies. The pin/laminate interface was modelled with a user defined constitutive cohesive-friction law, which was implemented by a VUINTERACTION subroutine[3]. In the subroutine, a modified Coulomb friction formulation, which was proposed by considering the Z-pin surface roughness, was coupled with a bilinear cohesive formulation to simulate pin/laminate bonding and pin/laminate frictional pull-out [3,4]. The simulations are firstly verified against experiments in terms of both global and local observations. The high-fidelity modelling technique is then used to unveil the bridging mechanics of discrete through-thickness reinforcement in curved laminates when subjected to an ambient through-thickness tensile stress field.

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Probability Distributions of Mechanical Properties for 2D-C/SiC Composites under Uniaxial Tensile

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Key Words: *CMCs, C/SiC, Damage Evolution, Meso-model, Uncertainty*

C/SiC ceramic matrix composites (CMCs) are one of the most important materials for aerospace thermal protection structures due to their excellent properties, such as high temperature resistance, high specific strength and high specific modulus. However, the complex manufacturing process leads to the inevitable emergence of initial defects in the matrix and oxidative damage of the fiber bundles, which may result in the complicated microstructure of the materials and significant decrease in the mechanical properties of C/SiC composites. Hence, it is of great importance to find the internal damage behaviours of C/SiC composites and to construct the suitable mechanical constitutive of materials for the structural analysis and design.

In this paper, the probability distributions of mechanical properties for 2D-C/SiC composites under the uniaxial tensile are focused on. The representive volume element (RVE) model of 2D-C/SiC composites in meso-scale was established by TexGen, and the periodic boundary conditions were imposed to predict the initial elastic properties of the composites. Uncertainties of the tensile strength and elastic modulus were considered to model the random features of fiber bundles and matrix and to quantificate the uncertainty propagation of mechanical performance of composites. The input probability distributions and their parameters are obtained from statistical data of experiments, and normal and Weibull distributions are applied to modulus and strength, respectively in this research. The progressive damage analysis under uniaxial tensile was conducted with finite element method (FEM) through user-defined subroutine considering multi-failure modes of fiber bundles and matrix, whose results show good consistency with those of the experiment. 100 repeated FEM simulations were performed with independent random sampling of input parameters, to characterize the randomness of mechanical properties of materials reasonably, which demonstrates the validity of the proposed model for performance prediction and structural analysis of 2D-C/SiC composites inconsideration of initial uncertainties.

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Versatile Fatigue Life Evaluation of CFRP Laminates Based on Interfacial Normal Stress

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Key Words: *Carbon fibers, Fatigue, Finite element analysis, Fractography, Life prediction*

Fatigue life is one of the most important strength factors to be considered in the equipment design. For metallic materials, a design method has been established to determine the allowable stress obtained from specimens and to complete the design after confirming that the stress is below the allowable value, as shown in the technical standard for high pressure vessels.

In the case of carbon fiber-reinforced plastics (CFRP), fatigue design has not been established to guarantee the long-term reliability required for application to strength members, because the complex fracture processes due to the microstructure of CFRP have prevented the application of established methodologies for metallic materials. To ensure the long-term reliability of CFRPs, it is necessary to perform a long-term endurance test that imposes actual loads on actual parts, as executed in the design verification test of the high-pressure hydrogen storage tank for fuel cell vehicle. In order to break away from this situation, it is necessary to establish a fatigue life evaluation method for CFRP equipment with highly versatile parameters.

The authors proposed the fatigue life evaluation method of unidirectionally (UD) reinforced CFRP specimens from the fatigue test results of the pure resin constituting CFRP [1]. Based on the assumption that the fatigue life of CFRPs is governed by that of its matrix resin, the interfacial normal stress (INS) obtained from micro-scale stress analysis is used as an evaluation index. INS, which was proposed by Hojo et al. [2], is defined as normal stress on a plane perpendicular to a line of minimal length that connects the center axis of carbon fibers.

In this study, we evaluate the applicability of the INS evaluation method to CFRP laminated specimens, since the previous study has been performed only for UD specimens. Three types of laminated specimens with different lamination configurations ($[0/30/-30/90]_s$, $[0/45/-45/90]_s$, and $[0/60/-60/90]_s$) were prepared and fatigue tests were conducted in advance.

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Fatigue Behaviour of Open-hole Carbon Fibre/epoxy Composites Containing Electrospun Nano-modified Diels-alder Based Resin Interleaves as Self-healing Agent. Experimental Campaign and Numerical simulation

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Key Words: *CFRPs, Self-healing, Electrospinning, Open hole, Fatigue, Tensile, Diels-alder, GNPs, numerical simulation*

Diels-alder (DA) based polymers exhibit healing functionalities on polymer level due to their thermal reversible nature [**1**]. In the current investigation, self-healing (SH) resin based on Diels-Alder (DA) reaction mechanism was integrated into high performance aerospace carbon fiber reinforced plastics (CFRPs) by electrospinning process technique (solution and melt electro-writing process). The effect of the selected SHA into CFRPs was further assessed. More precisely, open-hole reference and SHA modified CFRPs (containing GNPs at the amount of 1 wt %) coupons have been tested under quasi static tensile and tension-tension fatigue loading conditions. Their stacking sequence was $[45/-45/0/90]_{2S}$ and had similar fiber volume fractions. The structure of the experimental test campaign organized and realized for the needs of the current work as follows. The work started with tensile tests to pristine and open hole CFRPs coupons (for both reference and modified) in order to identify the apparent modulus and the ultimate tensile strength (UTS). Also, we had to investigate whether the introduction of the SHA into the structure of CFRP has any knock down effect to the mechanical properties. Then, the fatigue procedure followed and divided into three stages. The first stage investigates the fatigue life performance of reference and SHA modified CFRPs at continuous fatigue loading conditions. In the second stage, the fatigue experiments for both reference and modified composites were paused every 10 k cycles in order the damage evolution within the composite to be monitored using c-scan inspections. Finally, during the third stage the same route as in the second study level was followed, together with the activation of the healing process after each interruption of fatigue loading. Thus, this investigation thoroughly investigates the effect of the SHA healing capacity on the fatigue life performance of CFRPs. All tests were conducted under load amplitude control at 0.8 of UTS of reference CFRP, at R=0.1 and loading frequency f =5Hz. According to quasi static experimental results, it was shown that the incorporation of the SHA did not significantly deteriorate the in-plane mechanical properties of the entire composite. The activation of the healing functionality of modified composites at certain number of fatigue cycles revealed damage recovery based on c-scans (macroscopically) which further improved the mechanical performance of the composites. For all fatigue tested material sets a three-stage pattern of stiffness degradation was observed. Furthermore, numerical modelling and simulation of damage tolerance and healing capability of these CFRPs were performed via the development of appropriate cohesive zone models. The constitutive behavior of the cohesive zone was defined by the traction–separation relation derived from laboratory tests. The variation of the traction-separation relation after healing is directly related to the nature of SH material.

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Finite Element Analysis of Repeated Damage and Healing Behavior in alumina/SiC Composite Ceramics

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Key Words: *Self-healing ceramics, Finite element analysis, Oxidation kinetics, Constitutive model*

Unexpected and unstable rapid crack growth among various damage developments is a serious problem for brittle materials. Therefore, it is useful to improve the reliability by adding the self-healing function to those materials, such as concrete, glass, and ceramics. Among them, self-healing ceramics, which can automatically repair micro cracks by using the oxidation reaction, are attracting attention. The mechanism of crack-repairing in ceramics imitates healing process of human bones. For example, alumina (Al_2O_3)/silicon carbide (SiC) particle composites is a typical self-healing ceramics [1]. In this material, when the crack occurs, SiC particles (self-healing agent) combined in Al_2O_3 matrix react with oxygen in atmosphere and change to silicon oxide (SiO_2). Then, the oxides fills up cracks by volume increasing. It has been clarified that the Al_2O_3/ SiC composite material is an excellent material system that can simultaneously achieve crack filling and high strength of the healing part [2]. However, for the evaluation of self-healing materials, unlike ordinary materials, novel numerical analysis methods to evaluate both the damage and healing processes as reciprocally continuous processes need to be developed. Under such circumstances, recent developments have been observed in formulating both damage and healing processes within the framework of the continuum damage mechanics [3].

In this study, we conducted the finite element analysis of Al_2O_3/SiC composite self-healing ceramics by using the damage-healing constitutive model based on the oxidation kinetics [3]. To verify the effectiveness of the constitutive model and analysis scheme, we used specimens with a chevron notch for the three-point bending test, which can suppress rapid fracture of cracks even in materials with low toughness. Then, we demonstrated the analysis results of repeated damage-healing processes within the framework of finite element method. It was confirmed that the present finite element analysis (FEA) methodology could reasonably reproduce the basic characteristics of strength recovery in self-healing ceramics. Thus, we concluded that the present FEA methodology can be used for studying the self-healing behavior linked with the microstructure distribution and fracture properties, which is essential for the mechanical and material design of self-healing ceramics.

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Low-Velocity Impact Damage and Intrinsic Healing in Fibre Reinforced Polymer Composites

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Key Words: *low velocity impact, fibre reinforced polymer composite, micro-damage, intrinsic self-healing, micromechanical constitutive model, Abaqus/Explicit*

A micromechanics-based constitutive model for fibre reinforced polymer composites with intrinsic self-healing ability is presented in this work. Homogenisation is carried out using the Rule of Mixtures (ROM), i.e. equations defining mechanical properties of the homogenised composite. On the other hand, the Voigt (iso-strain) and Reuss (iso-stress) approximations are used as a means for localisation.

At the micro-scale, matrix constituent is modelled using the previously developed constitutive model comprising micro-damage-healing model and the isotropic hardening plasticity model described and validated in [1]. In this model, the effect of micro-damage on the matrix material is represented as deterioration of the elasticity modulus, whereas the healing phenomenon represents its recovery. Furthermore, the reinforcing fibres are modelled as transversely isotropic linear elastic material with Hashin fibre failure criterion and progressive fibre damage. The model was implemented in Abaqus/Standard user material subroutine UMAT and validated for static loading cases in [2].

The model is implemented into the Abaqus/Explicit user material subroutine VUMAT. Moreover, it is validated using low-velocity impact tests. Experimental results are taken from [3] where composite specimens consist of woven glass fibres as reinforcement and an epoxy-thermoplastic blend as the matrix constituent. The blend consists of diglycidyl ether bisphenol A (DGEBA) epoxy resin and poly($\boldsymbol{\varepsilon}$-caprolactone) thermoplastic polymer. Numerically, the warp and weft yarns are treated as unidirectional plies.

The model proves to be applicable for simulation of healing phenomenon after low-velocity impact damage in woven composite structures. Finally, the model could describe healing behaviour of other types of intrinsically self-healing composites if appropriate constitutive material laws are applied.

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Toughening and Healing of CFRPs by Diels-alder Based Nano-modified Resin through Melt Electro-writing Process Technique. Experimental Campaign and Numerical simulation

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Key Words: *CFRPs, Self-healing, Melt Electro-writing, Diels-alder, Mode I, GNPs, Numerical simulation*

In the present work, a novel approach in terms of self-healing agent (SHA) incorporation into uni-directional carbon fiber reinforced plastics (CFRPs) has been demonstrated. More precisely, healable resin based on Diels-alder (DA) reaction mechanism, containing or not graphene nanoplatelets (GNPs) at the amount of 1% wt, was integrated locally into the mid-thickness area of CFRPs. The procedure was performed by the melt electro-writing process (MEP) technique. DA-based polymers present resin type behavior, while are mendable and present healing functionality through heating upon their melting point (T_m) temperature [**1**]. MEP is a processing technique for producing fibrous structures from polymer melts [**2**]. In this case of electrospinning technique, the collection of the fiber can be very focused. Therefore, combined with moving collectors, MEP is a way to perform 3D printing with ultrathin fibers. In our case, ultrathin fibers of DA resin were directly printed on the surface of CFRP pre-preg plies. Based on this, reference and modified CFRPs with (a) pure SHA and (b) SHA containing 1% wt GNPs were manufactured for the needs of the current study and further tested under Mode I loading conditions. Based on experimental results both types of modified CFRPs exhibited considerable enhancement of the fracture toughness properties with GNP modified ones to exhibit the best toughening performance (G_{IC} value was increased by almost 280%). After Mode I testing, the damaged samples passed through the healing procedure and then tested again under Mode I loading conditions. After repeating of the tests, acceptable healing efficiencies were achieved (up to 50%) as part of the fracture toughness properties were restored. GNP modified ones exhibited the best healing behaviour. Furthermore, numerical modelling and simulation of damage tolerance and healing capability of these CFRPs was performed via the development of appropriate cohesive zone models. The constitutive behavior of the cohesive zone was defined by the traction–separation relation derived from laboratory tests. The variation of the traction-separation relation after healing is directly related to the nature of SH material. This approach provides a robust numerical tool for the design of composite structures that include self-healing sites. Based on that, it was shown that simulated and measured R-curves are in good agreement. Finally, optical microscopy examinations not only showed that the epoxy matrix at the interface is partly infiltrated by the DA polymer, but it also revealed the presence of pulled out fibres at the fractured surfaces, indicating ductile behaviour due to SHA presence.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Lateral Resistance of Buried Pipes by Frictional Limit Analysis

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Key Words: Burried pipes, Limit Analysis, Friction, Porous materials

Pipelines are vital means of transportation of liquids and gases over large geographical areas. Regarding hydrocarbons, they must be flow at high pressure and temperature to avoid wax formation. Low temperatures may lead to deposits at pipe walls, increasing the pressure or blocking the fluid flux. Under such thermal and mechanical loads and Poisson's effect, the pipe tends to expand longitudinally. Since longitudinal movements are restricted, high compressible forces are developed, leading to buckling occurrence if a critical value is reached. The occurrence of lateral buckling strongly depends on the surrounding soil, friction at pipe-soil interface, pipe diameter and buried depth and subsoil characteristics [1]. Then, the evaluation of soil lateral resistance that will entail an imminent breakout is important.

This work aims the analysis of the soil lateral resistance under limit analysis formulation considering friction at pipe-soil interface. Limit analysis is a direct method, posed as an optimization problem with constraints, and aims the determination of the collapse power of an elastic perfectly-plastic body and do not consider the load history. In this approach, the pipe is considered as a rigid body while the soil mass is a deformable one. Then, at imminent plastic collapse state, the contact between the rigid and deformable bodies is assumed as known, with permanent contact at normal direction and a slipping rule at tangential direction. Coulomb friction law is considered. The limit analysis problem is solved by a quasi-Newton algorithm and a condensation technique allied to Lemke algorithm is used to solve the complementarity problem at contact. The cohesive soil mass follows the yield criterion proposed by [3], derived from homogenization theory considering cohesion, material internal friction and porosity.

The soil lateral resistance is evaluated by limit analysis considering friction at soil-pipe interface and porosity of soil mass, discretized by finite elements and under plane strain hypothesis. As results, the soil resistance forces per length, the velocity and stress fields at soil mass are determined as well as the slip lines.

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Modeling Dynamic Ductile Fracture and Thermal Softening With a Variational Phase-Field Framework

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Key Words: fracture, phase-field, dynamics, plasticity, shear bands

We propose a model to simulate dynamic ductile fracture based on a variational phase-field framework. In this framework, a coalescence dissipation term couples plasticity and fracture by degrading the fracture toughness as the equivalent plastic strain increases [1]. Compared to other models that degrade the plastic energy with damage, the current model avoids crack growth through plastic zones in compression and relaxes the upper bound on the regularization length. In addition, the variational framework allows for the consistent inclusion of plastic dissipation in the heat equation as well as thermal softening. Results from various benchmark problems in dynamic ductile fracture are presented to demonstrate the capabilities of the model. In particular, we demonstrate how the model is capable of capturing high strain rate effects such as brittle to ductile transitions and shear band formation. Importantly, these phenomena are naturally captured through the physics in the model, without the need for phenomenological criteria such as stability thresholds for the onset of shear band formation.

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Numerical Simulation of Neck Propagation in Double Network Hydrogel

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Key Words: Neck Propagation, Hydrogel, FEM, Nonaffine Polymer Chains Network Model

Double network (DN) hydrogels have drawn much attention as an innovative material having both high water content and high mechanical strength and toughness. Futhermore, yielding phenomenon was observed in some tough DN gels[1]. For example, on tensile tests of DN gels that made from relatively sparse first networks, narrow zones appear in the sample and grow up with further stretching. During the neck propagation, a plateau region appears in the loading curve. The plateau value of the tensile stress hardly depends on the stretching rate. After the neck propagation, the gel becomes fairly soft, showing an elastic modulus *ca*. 1/10 of the virgin sample, and sustains large elongation, up to an elongation strain of around 20. The observations on the softened gels after the tensile test demonstrate that irreversible structural change takes place inside the gels, although their appearance is almost unchanged.

In this study, we at first employ a nonaffine polymer chains network model[2] to account for such irreversible structural change during the deformation of DN gels. And then, a finite element model of the DN gels under simple tension is constructed. On the other hand, neck propagation is one kind of localized instability and there will be a local transfer of strain energy from one part of the model to neighboring parts. This class of problems has to be solved either dynamically or with the aid of (artificial) damping; for example, by using dashpots. Fortunatly, Abaqus/Standard provides an automatic mechanism for stabilizing unstable quasi-static problems through the automatic addition of volume-proportional damping to the constructed model and the applied damping factors can vary spatially and with time to account for changes over the course of a step, where the damping factor is controlled by the convergence history and the ratio of the energy dissipated by viscous damping to the total strain energy. Furthermore, Abaqus/Standard can reduce the time increment to permit the process to occur without the unstable response causing very large displacements.

The simulation results show that the nonaffine polymer chains network model can be employed to reproduce neck propagation in DN gels very well.

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Applicability of Modified von-Mises Damage Criterion to Compressive Fracture Behaviour of Cement-Based Materials

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Key Words: *Modified von-Mises criterion, Damage Model, Compressive Fracture, Crack Growth, Cement-Based Materials*

The Applicability of the damage model based on the modified von-Mises criterion [1] is studied for compressive fracture behaviour of cement-based materials such as mortar and concrete. Two numerical experiments of mortar plates with a circular hole under compression are presented, and the results are compared with experimental results to demonstrate the applicability of the modified von-Mises criterion for compressive fracture behaviour.

We first show the formulation of the damage model based on fracture mechanics of concrete [2]. The damage model evaluates the generation and propagation of cracks by using the modified von-Mises criterion. Cohesive crack growth in cement-based materials can be represented by introducing the traction-separation law based on the fracture energy into the damage model. The fracture simulation of cement-based materials involving cohesive crack growth is performed in the non-linear finite element framework.

The crack propagation behaviour simulated with the modified von-Mises damage model is compared to existing experimental results. The comparison shows that the numerical results are in good agreement with the experimental results. This implies that the damage model with the modified von-Mises criterion allows the simulation of cohesive crack growth in cement-based materials subjected to compressive load. To verify the capability for simulating the compressive fracture behaviour quantitatively, the numerical results are also compared to our own test results with the DIC measurement. From these results we confirm that the damage model with the modified von-Mises criterion is applicable to the crack propagation analysis of cement-based materials subject to compressive load.

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Collapse Simulation of Concrete Structure Considering Contact between Masses Generated by Crack Penetration Using RBSM

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Key Words: *RBSM, Cracking, Collapse simulation, Geometric nonlinearity, Contact problem*

In order to accurately reproduce the collapse behavior of concrete structures, an algorithm to update the network between elements is introduced in the Rigid-Body-Spring Model(RBSM) considering geometric nonlinearity [1][2]. Specifically, a new network was constructed by placing multiple contact-determining spheres on Voronoi polyhedral elements and a reduced integration Timoshenko beam element between the newly-determined contact elements. As a result, in the numerical simulation of concrete structures, a contact phenomenon after large displacement and large rotation behavior, which could not be reproduced by the conventional RBSM, can be reproduced.

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Ductile Fracture Initiation and Propagation Using Gurson-Cohesive Model (GCM) in 3D

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Key Words: *Ductile fracture, Computational mechanics, Crack initiation, Crack propagation, Gurson, Cohesive zone model*

For the computational simulation of ductile fracture associated with void growth and coalescence, various computational methods have been developed [1]. However, most computational methods such as continuum damage models suffer from mesh dependent issues, and thus a regularization term and/or a length scale parameter is introduced to alleviate the mesh dependency. In this study, the Gurson model and cohesive zone model are integrated to reproduce ductile fracture behaviors [2]. The transition from the plastic deformation to the cohesive fracture is linked using the porosity-based crack initiation criterion in conjunction with the stress triaxiality. The Gurson-Cohesive model (GCM) is validated using experiments performed by Sandia National Laboratory [3]. Both tensile coupon tests and compact tension tests are investigated with the same material properties within the unified computational framework. The computational results reproduce the engineering stress-strain curve and the area reduction ratio for the tensile coupon test. The proposed framework captures the load versus crack opening displacement relations for the compact tension tests with three cases of the initial notch length. Furthermore, the computational results converge under mesh refinement without introducing any regularization term and/or length scale.

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Iterative Simulation of Fractures in Brittle Solids using Multi-sphere DEM

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Key Words: *fractures, discrete element methods, strain energy field, sintered materials.*

Discrete Element Methods (DEM) are good alternatives to FEM for the study of fractures in brittle solid materials [1]. However, their precision is limited by the size of the elements used to represent the material. Hereby we study fractures in brittle materials by using smaller discrete elements just on the places where stresses are closer to the breaking thresholds. The solid material is divided into three-dimensional random Voronoï cells, and each cell, each of them a discrete element, is represented by a frozen clump of overlapping spheres [2]. If two cells share a face, the spheres of one cell in contact with those of the neighbouring one are joined across the face with rigid bars [3]. The forces and torques of such bars are used to compute the strain energy field, who has shown to be adequate to account for fractures in granular media [1]. Once the material is charged with an external load, only discrete elements with high strain energy fields are subdivided into smaller elements, who re-establish bonds between them and with all neighbours. The process is repeated until the desired resolution is reached, and then those bonds above a threshold are broken. In this presentation we show how the fracture surface can be retrieved with high accuracy and low computational costs, and the results are compared to continuum methods like FEM.

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Characterization of Finite Strain Elastic-Plastic Crack Propagation using Redefined J-Integral and J-Integral Range ΔJ

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Key Words: *Instructions, Multiphysics Problems, Industrial Applications, Covid-19*

In the present investigation, the crack propagation phenomena of 1TCT specimen made of stainless steel (SUS316) under large magnitudes of monotonic and cyclic loads are presented. The specimens experienced large deformations. In order to characterize the crack propagation, the J-integral [1] and the J-integral range ΔJ [2] have been adopted. It is, however, noted that the applications of the J-integral and the ΔJ were limited in infinitesimally small deformation problems. For example, Okada et al. [3] performed two-dimensional analyses under the assumption of infinitesimally small deformation. The fracture parameter T_ε^* -integral was proposed. It was defined as an integral on an infinitesimally small contour Γ_ε surrounding the crack tip. T_ε^* measures the deformation energy dissipating into the small region (process zone) V_ε surrounded by Γ_ε per unit crack extension. For the numerical computation, the T_ε^*-integral is written as a combination of far field contour and area integrals. Arai et al. [4] redefined the three-dimensional J-integral using the domain integral representation as an extension of the T_ε^*-integral to three-dimensional and finite strain elastic-plastic problems. It measures the energy dissipating into a small volume V_ε^o per unit crack extension. Then, the ΔJ was proposed by its extension to cyclic load problem (Arai et al. [5]).

In the presentation, the applications of the newly redefined three-dimensional J-integral and ΔJ to the fracture problems involving finite strain elastic-plastic deformation and cyclic load will be discussed. The experimental data of the JWES database [6] was used as references for the finite element analyses.

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Comparison of residual stresses of stainless steel between electron beam welding and conventional welding

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Key Words: *Welding, Residual stress, Electron beam welding, Stainless steel*

The high residual stress on the surface of the canister has a great influence on the occurrence of Chloride-Induced Stress Corrosion Cracking (CISCC). In conventional welding for stainless steel Post-Weld Heat Treatment (PWHT) cannot be performed, resulting in high residual stress. Since electron beam welding is known to have a smaller Heat Affected Zone (HAZ) width compared to conventional welding, applying electron beam welding to canister is expected to reduce residual stress and reduce the occurrence of CISCC.

Purpose of this study is to compare the residual stress distribution of a mock-up canister (Sandia National Laboratories Mockup canister) manufactured by conventional welding (Submerged Arc Welding, SAW) with the residual stress distribution when the conventional welding is replaced with electron beam welding. Electron beam welding was applied to the canister through finite element analysis using ABAQUS. The component was made from 304L stainless steel (SS). The analysis was carried out using uncoupled thermal and mechanical finite element analysis. Three-dimensional (3D) finite element models were used to simulate thermal and mechanical analysis. Thermal analysis was performed by simulating a moving cylindrical heat source. Stress analysis was performed using the results of thermal analysis and residual stress was calculated. The residual stress calculated through this analysis was compared with the residual stress measured by Sandia National Laboratories for a canister manufactured by conventional welding (SAW).

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Crack initiation prediction for high strength steel thin plate using simplified stress triaxiality-lode parameter damage model

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Key Words: *High Strength Steel, Ductile Fracture Criterion, Stress triaxiality, Lode parameter*

The use of high-strength steel in automobile manufacturing processes is increasing to reduce the durability and weight of automobile bodies and chassis. High-strength steel has higher strength than conventional materials, but has less ductility. Therefore, it is very sensitive to cracks occurring in cold processing processes, such as microcracks, which may cause damage or defects, especially in trimming or shear or punching processes. Defects caused by microcracks such as edge cracks are a very serious problem in product quality and productivity. Therefore, predicting the fracture of thin plate is a very important problem.

In predicting the ductile fracture of metals, many ductile fracture criteria have been proposed. McClintock, Rice, and Tracey argued that stress triaxiality is an important factor influencing the nucleation, growth and coalescence of microscopic voids and the ductile fracture criterion was presented as a function of stress triaxiality [1,2]. Xue and Wierzbicki confirmed through various experimental results that the Lode Angle parameter had a mutual effect on the initiation of ductile fracture like stress triaxiality [3, 4]. Bai and Wierzbicki modified the Mohr-Coulomb (MMC) criterion to predict many different types of specimen fracture under various stress triaxiality and lode angle parameter [5].

Previous ductile fracture criterion such as MMC model have many parameters and it is hard to decide the parameters. In this study, previous ductile fracture criterion using stress triaxiality and lode parameter was simplified. The constant of the simplified model was determined using tensile test specimen and SENT specimens which have two different notch radii for JSC 590 and JSC 980 materials. In addition, the validity of the proposed model was verified by applying the simplified model to the DENT specimens.

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Crack Propagation Criterion for a Pipe under Bending and Torsion Loadings

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Key Words: *Finite element analysis, Bending, torsion, Multiple loads, Stress triaxiality, Equivalent plastic strain*

In the previous study[1][2], ductile crack propagation behavior was reproduced by results of Central Research Institute of Electric Power Industry (CRIEPI) [3] under monotonic and cyclic loading bending tests for pipes installed in a light water reactor plant. It is also concluded that the crack propagation conditional equation with parameters of stress triaxiality and equivalent plastic strain proposed by Kumamoto[1] and Ohbayashi[2] can be reproduced.

As mentioned above, the analyses are reproduced from four-point bending tests under monotonic and cyclic conditions. On the other hand, experiment results subjected to multi-axial loads including bending and torsion are very few examples in order to ensure the validation of proposed criteria.

Recently, the CRIEPI conducted an experiment under combined bending and torsion on stainless pipe. The results are evaluated using numeriacl simulations by several organaizations and are checked in a round-robin analysis to ensure the validity of the results.

In this study, FE models are generated on 20 mm diameter stainless steel pipes with through-wall crack under combined bending and torsion and are simulated including ductile crack propagation. In addition, Otsuka et al.[4] have suggested that an increase in stress triaxiality accelerates the extension rate of voids and decreases plastic strain of ductile fracture. Therefore, it is reasonable to propose an equation using these parameters. Crack propagation criterion will be proposed using those results and are evaluated the validity of the criterion.

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Development of XFEM-based system for fatigue crack propagation analysis and its verification

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Keywords: *XFEM, Fatigue crack propagation, Stress intensity factor*, *Paris's law*

In this study, a system referred to as *sim2d* for fatigue crack propagation analysis based on extended finite element method (XFEM), which can model crack independently of finite elements, has been developed. This system employes an in-house XFEM code referred to as *NLXFEM3Dstruct* [1] and python scripts to control the code execution. A fatigue crack propagation analysis of a carbon steel compact tension specimen has been performed by the developed system as a verification. In this presentation, the analysis results by *sim2d* including the relationship between the crack length and the number of load cycles are compared with the results obtained by conventional finite element method (FEM), which requires re-meshing on each analysis step for crack propagation, and the reference solution in accordance with ASTM standard [3].

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Dynamic failure simulation of metal materials and structures under blast and impact loading

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Key Words: *Dynamic failure, Fracture, Shear band, Numerical simulation*

Studying the dynamic failure laws of metal materials and structures under blast and impact loading by numerical simulation is of great significance for characterizing the damage effects of explosive shock and designing novel impact-resistant structures. The metals' failure under strong dynamic loading involves multiple complex physical processes, such as the large deformation, the thermal-mechanical coupling, and the material state changes. These complex physical processes bring great challenges to numerical simulation, including the geometric description of complex dynamic failure modes such as cracks and shear bands, the determination of failure criteria, and the description of plasticity-damage coupled evolution, etc. In response to these challenging issues, a theoretical and computational thermal elastic-plastic phase field model is established based on the energy variational principle to describe metals' dynamic failure. The model realizes a unified description of the crack and shear band, and its efficient explicit finite element solved strategy is proposed. The model is further applied to three typical metals' dynamic failure issues under blast and impact loading: the transition of brittle and ductile failure modes of metals, the self-organization of adiabatic shear bands (ASBs), and the transition of failure modes of thin-walled disks under shock waves. This verifies the accuracy of the theoretical model and the robustness of the computational model. This work lays the foundation for the subsequent development of damage assessment and protective structure design for blast and impact loading based on simulation.

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Fracture Mechanics in Three-Dimensional Isogeometric Models: Evaluating J-Integral as a Post Isogeometric Analysis Calculations

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Key Words: *Isogeometric Analysis (IGA); Fracture mechanics; Three-dimensional; Stress singularity; Stress Intensity Factor (SIF)*

A study on J-integral computation for three-dimensional Isogeometric Analysis (IGA) has been conducted. IGA is a novel analysis method that has been investigated by researchers and engineers in the last decade. IGA was initially developed and presented by Hughes et al. [1]. One of the possible applications of IGA is fracture mechanics. In fracture mechanics, accurate evaluations of Stress Intensity Factors (SIFs) are very important. In the applications of the Finite Element Method (FEM), two-dimensional J-integral by Rice [2] has often been used to evaluate the SIFs. The extension to three-dimensional was carried out by Blackburn[3] and Kikuchi et al. [4]. The domain integral method for three-dimensional J-integral was presented by Li et al. [5]. In this study, a domain integral method suited for IGA is presented. In the present IGA, the second order B-spline and Non-Uniform Rational B-Splines (NURBS) functions are adopted as basis functions. A singular patch method to express the singular stress field in the vicinity of the crack front following the idea of Barsoum's quarter-point finite element [6]. Examples of embedded and surface elliptical cracks to demonstrate the accuracy of the proposed J-integral are presented.

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Proposal of Crack Propagation Criterion Considered Constraint Effect under Extremely Low Cycle Fatigue; Evaluation by 1.5T-CT Specimen

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Key Words: *Extremely low cycle fatigue, Fracture criterion, Constraint effect, Finite element analysis, Stress triaxiality, Equivalent plastic strain increment*

The prediction of fracture behavior under extremely low cycle fatigue due to excessive loading is necessary for the life assessment of structures. ΔJ criterion has been used to assess the life under low cycle fatigue. However, the applicability of this method is not well confirmed under extremely low cycle fatigue. Fracture toughness is dependent on the loading conditions and geometry due to the constraint effect.

In the previous study [2], a crack propagation criterion was proposed for a 1T-CT specimen of SUS316, focusing on the physical quantities near the crack tip. These are the stress triaxiality and the equivalent plastic strain increment. The former is a parameter related to the growth of voids in ductile fracture, while the latter is a parameter that indicates the degree of plastic deformation. However, no comparison has been performed for specimens of different shapes or materials, and more detailed verification is required.

The objective of this study is to evaluate the validity of the crack propagation criterion proposed in the previous study [2] by applying it to CT specimens of different thicknesses and materials.

In this study, two types of crack propagation simulations were performed on a 1.5T-CT specimen of SGV410 under extremely low cycle fatigue fracture tests using the finite element code, ANSYS. The first one is generation phase simulation. In the simulation, the physical quantities near the crack tip were obtained and the parameters of the crack propagation criterion were identified. The second one is the validation phase simulation, in which the crack propagation criterion is used as the crack propagation criterioin to evaluate whether the experimental crack propagation behavior can be reproduced.

The results of both the generation phase simulation and the validation phase simulation are in good agreement with the experimental results.

We'd like to disscuss the accuracy of prediction by the proposed crack propagation criterion under extremely low cycle fatigue.

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Proposal of Crack Propagation Criterion Considered Constraint Effect under Extremely Low Cycle Fatigue; Evaluation by 1T-CT and 2T-CT Specimen

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Key Words: *Extremely low cycle fatigue, Finite element analysis, Constraint effect, Fracture criterion, Stress triaxiality, Equivalent plastic strain increment*

It is important to understand unstable fatigue fracture mechanism because fracture accident is occupied fatigue 80% of the total [1]. However, a highly reliable evaluation method for under extremely low cycle fatigue caused by earthquakes has not yet been developed because of variable fracture toughness due to the constraint effect with large deformation.

Crack propagation criterion proposed in the previous study was validated under restricted condition [2], however it wasn't considered constraint effect. The objective of this study is the proposal of crack propagation criterion considered constraint effect under extremely low cycle fatigue.

As a matter of procedure, we model compact tension specimen finite element it was used in the previous study changed the thickness which is one of the constraint effect. And then after analysis which simulates behavior based on the experiment, we conducted validation applied crack propagation criterion which was proposed in previous study.

As a result, analysis applied crack propagation criterion in the previous study was obtained good accuracy. Crack shape was formed following distribution of effective plastic strain in thickness dimension. As a reason for that contribution ratio of effective plastic strain in crack propagation criterion is higher than stress triaxiality. In the presentation, crack shape in the analysis will be discussed after re-examination the contribution ratio in physical quantities and the method of evaluation.

The crack propagation criterion in the previous study is confirmed validity in several cases of thickness. We'd like to discuss validity in cases of different material properties, specimen shapes and crack shape.

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A New Method to Identify Delamination Shape Using Topology Optimization and Visualization of Ultrasonic Waves

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Key Words: *Non-destructive Evaluation, Polymer-Matrix Composites, Delamination, Topology Optimization, Ultrasonic Wave Propagation*

This study proposes a new method to identify delamination shape in carbon-fiber-reinforced plastic (CFRP) laminates using topology optimization and visualization of ultrasonic waves. Although the technique to visualize ultrasonic wave propagation aids in detecting defects such as delamination, it is difficult to evaluate them quantitatively. The authors [1] proposed the topology optimization-based damage identification method combined with the technique and quantitatively identified the crack in a metal plate. Application of the proposed method to predicting critical damage in composite structures, such as delamination, will enhance structural reliability.

The concept of the proposed method is to estimate the defects as the distribution of 'damage parameters' that reproduces the experimentally visualized ultrasonic wave propagation on an inverse analysis model. In this study, delamination is modeled using cohesive elements [2] and is estimated as distribution of the internal residual strength variables that minimizes the error between the ultrasonic features obtained in the experiment and those in the finite element analysis.

To verify the feasibility of the present method, this study applied it to a cross-ply CFRP laminate with an artificial delamination. The stacking sequence of the specimen was $[0_4/90_4]_S$ and the artificial delamination was introduced by a 10×10 mm polyimide film at one of the two interfaces of the 0° and 90° layers. When the delamination identical to the specimen was developed by the cohesive elements and when the finite element analysis was performed under the same condition as the experiment, the maximum amplitude of the analysis was high within the delamination area, which was the same result as the experiment. Therefore, the optimal distribution of the internal residual strength variables can be estimated by minimizing the error between the maximum amplitude map acquired in the experiment and in the inverse analysis model.

Under the above-mentioned procedure, the shape of the artificial delamination was successfully estimated using the present method. The detailed results and discussion will be demonstrated in the presentation.

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Computational and analytical homogenization of creep in fiber reinforced metals

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Key Words: Shear lag modeling, Computational homogenization

In this presentation we revisit the well-known, one-dimensional shear lag model introduced by Kelly and Street [1]. Owing to it's simplicity, it is widely used in material sciences to assess and interpret experimental results. Originally the model was proposed to evaluate the stationary creep response of circular fiber reinforced materials with large fiber aspect ratios and low fiber volume fractions. Other applications include square fibers and cellular materials [2].
However, it is usually difficult to evaluate experimentally whether the model is appropriate for the given material, as morphology modification is limited due to strongly interrelating solidification and processing parameters and as test conditions are limited to uniaxial creep tests.
The goal of the present study is to use modern FFT-based solvers [3, 4] to evaluate the suitability of the Kelly-Street model for various materials with changing morphology (volume fractions and aspect ratios). Therefore we use artificially generated microstructures, which offer the flexibility of adjusting morphology. We evaluate stationary creep response and compare simulated results against Kelly-Street model predictions.
As will be shown, for certain fiber aspect ratios and volume fractions the Kelly-Street model fails to predict stationary creep accurately, which is linked to basic model assumptions. This observations motivates subtle, physically motivated modifications of the model. We will show, that the accuracy of Kelly-Street model predictions can be significantly improved, which allows future usage to obtain accurate estimates of creep behavior for various morphological features.

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Damage Propagation Analyses of CFRP laminate with impact damage under compressive load using Zig-zag CZM

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Key Words: *CFRP laminate, FEM, Damage propagation, Zig-zag CZM, Impact test, CAI test*

Due to high specific strength and stiffness, carbon fiber reinforced plastics (CFRP) have been widely used in aviation industries in recent years. However, CFRP laminate is susceptible to out-of-plane load, which can lead to complex damage such as delamination, matrix crack and fiber breakage. Because the damage may cause a decrease in compressive strength, CAI (Compression After Impact) strength is important in designing CFRP laminate structures.
In this study, Finite Element Method (FEM) is used for strength evaluation of structures. Interface elements considering Cohesive Zone Model (CZM) are introduced to model multiple delamination and matrix cracks of laminate. For nonlinear problem, such as evaluating damage propagation behavior of structures under large deformation, it is generally necessary to use explicit dynamic finite element analysis using mass scaling. However, in order to perform efficient analysis, it is worth studying implicit analysis using cohesive zone model considering Zig-zag softening law to improve convergence [1].
In this presentation, the implicit method is used to perform damage propagation analyses of CFRP laminates subjected to out-of-plane load, and subsequently subjected to compressive load. The results including size of damage in the impact test analysis and CAI strength in the CAI test analysis are compared with those of experiments performed by JAXA [2] and discussed.

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Damage Simulation for Textile Composites Using Fiber-bundles / Matrix-resin Separated Mesh

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Key Words: Finite element analysis, Damage analysis, Cohesive zone model, CFRP, Woven composites

In this study, the authors propose a novel progressive damage simulation method for textile composites. The method is based on finite element analysis in which fiber bundles and matrix resin are separately meshed. Two meshes are connected using cohesive zone model (CZM), which is also utilized to simulated interface damage between fiber bundle and matrix resin. Damage in the fiber bundle and matrix resin are simulated using continuum damage mechanics (CDM) model.

In the conventional finite element analysis of textile composites, the mesh must be divided along the interface between fiber bundles and matrix resin. The meshing process is often difficult and labor consuming because of the complex shape of textile microscopic structure. Moreover, textile structure often results in small, distorted resin elements surrounded by the fiber bundles. Such elements increase the calculation cost and reduce the calculation accuracy. In the proposed method, however, fiber bundles and matrix resin are separately meshed. Moreover, regular cubic grid mesh can be used for modeling matrix resin. It means that small, distorted resin elements are no longer necessary, and element division process becomes much easier.

In the presentation, formulation of the proposed method will be presented first. Progressive damage simulation analysis for simple textile composites will then be performed using the proposed method, and the results will be compared with those of conventional damage simulation for validation of the method. Calculation costs will be compared for demonstrating the effectiveness of the proposed method. Finally, progressive damage simulation for 3-dimensional woven composites, which have complex textile microscopic structure, will be presented for demonstrating the effectiveness of the proposed model.

Development of a Novel Element for Simulating CFRP Strength Deterioration due to Cyclic Loadings Based on Entropy Damage

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Key Words: *FEA, Strength deterioration, Cyclic loading, Hashin criteria, Entropy damage*

We developed a novel element for finite element analysis to simulate strength degradation of CFRP under cyclic loadings. The failure criterion is based on Hashin criteria [1]. The six types of strengths in Hashin criteria: fiber directional tensile, fiber directional compressive, transverse tensile and transverse compressive, fiber axial shear, and transverse shear strengths, are degraded respectively, depending on corresponding cyclic loadings. It is to say, damage initiation criteria change with respective cyclic loadings. The issue attributes to how the strength degrade in response to the cyclic loadings.

CFRP consists of elastic fiber and viscoelastic matrix so CFRP possesses viscoelastic characteristics more or less. The dissipated energy due to viscoelastic behavior is divided by absolute temperature, which becomes entropy increase. The entropy increase directly relates to the damage of material [2]. Sato et al [2] predicts residual strength of CFRP after some loadings, utilizing entropy damage criterion which is calculated based on viscoelastic constitutive equation of polymer resin. This criterion is applied in this study.

The orthotropic viscoelastic constitutive equation is assumed in this study. The viscoelastic model is expressed by general spring and dashpot systems. Depending on loading history including cyclic loadings, both springs and dashpots move. The work for movement of dashpot corresponds to dissipated energy so entropy increase can be identified always. The strengths in Hashin criteria are degraded according to the entropy increase. The entropy increase consists of amount of each directional dissipated energy divided by absolute temperature.

In respect to damage evolution, the energy release rate is also degraded according to the dissipated energy, even after damage initiation. Therefore, during damage evolution traction separation behavior becomes nonlinear. ABAQUS user subroutine is employed in this study. Thus, we have developed a novel element which can simulate deterioration caused by essentially various loadings.

The element can simulate not only strength degradation caused by monotonic cyclic loading, but also various cases such as stress level, frequency, stress ratio, even temperature changes. Hence, the element can be inherently used universally for long-term durability of CFRP. Some application examples are shown in this presentation.

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Direct FE^2 – Concurrent multiscale and multiphysics modelling of composites with ABAQUS

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Key Words: *Multiscale, Multiphysics, Transient analysis, Structural finite elements*

FE^2 offers an attractive approach to finite element analysis (FEA) of composites because it is often difficult to obtain accurate homogenized constitutive relations due to complex microstructures and the nonlinear interactions among the constituents of the composites. Homogenized properties are obtained through FEA of representative volume elements (RVE) where the different phases of the composite are explicitly modelled. However, the conventional implementation of FE^2 requires familiarity with computational homogenization and some in-house coding. The RVE calculations need to be carried out in tandem with the FEA of the composite structure with constant information exchange between the micro and macro scale simulations. We recently proposed a much simpler implementation - Direct FE^2 - that enables FE^2 to be carried out on commercial FE codes with only two pre-processing steps [1]. This was demonstrated in an example of the deformation of a 2D composite beam cantilever beam with geometric and material nonlinearities using solid finite elements.

The implementation of Direct FE^2 for composite materials for other types of analyses will be presented. Leveraging on the capabilities of ABAQUS in thermal and transient analyses, we show how coupled multiscale thermomechanical problems can be solved [2] and how inertial effects can be incorporated at the microscale [3]. Direct FE^2 for beam and plate elements, which are important FEA of composite laminates because of their computational efficiency, is also presented.

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Dynamics of an Aircraft with Corrugated Morphing Control Surfaces

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Key Words: *Morphing Wings, Control, Flight Dynamics, Aeroelasticity*

Conventional aircraft wings have rigid control surfaces to control the aircraft flight, but those devices induce abrupt shape changes of the wing and gaps on the surface. Morphing technology, which enables smooth wing shaping, can improve the aerodynamic characteristics of the aircraft, and it has been extensively studied for the last decades.

A flexible structure that makes the smooth wing shape change possible is one of the key components of morphing technology. One of the promising structures is a corrugated structure. The morphing concept with corrugated panels has been investigated, which demonstrated that the corrugated morphing wing can improve the static aerodynamic performance and that it is a feasible morphing concept with a simple actuation system [1,2].

The aforementioned studies demonstrated the static aeroelastic characteristics of corrugated morphing wings, but the performance of the morphing aircraft remains to be investigated. Corrugated structures are very flexible, and the flexibility may affect the flight performance of the entire aircraft [3]. Detailed studies are needed to understand the flight characteristics with corrugated morphing control surfaces.

The objective of this study is to understand the influence of the flexible corrugated morphing structures on the flight dynamics of the entire aircraft. An aeroservoelastic simulation framework for corrugated morphing control surfaces has been developed combining a finite element method, an unsteady vortex lattice method, and a linear quadratic regulator. By coupling the rigid-body flight dynamic formulations with this framework, the flight motions of the morphing aircraft will be numerically simulated. The interactions between the rigid-body flight dynamics of the entire aircraft and the flexible corrugated morphing structures will be demonstrated in representative flight conditions.

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Exploring Direct FE2 in Modelling Heterogeneous Problems beyond Scale Separation

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Key Words: *Multi-scale, Micro-inertia, Dynamics, Heat transfer, Micromorphic*

FE2 is an appealing approach for efficient modelling heterogeneous materials with constituent properties compared with direct numerical simulation. But FE analyses at the macroscale and the microscale have to be performed in a nested manner. Direct FE2 recently proposed by Tan et al. [1] overcomes this deficiency through formulating a single FE analysis, in which both macro and micro DOFs are involved and coupled through kinematical constraints. Therefore, it can be directly implemented in existing FE software and largely simplifies the modeling. An underlying assumption of the classical FE2 or Direct FE2 is the separation of length scales, namely, the microscopic length is much smaller than the macroscopic characteristic length. However, this assumption may not always hold in advanced materials or structures, such as metamaterials and micro-devices.

In this presentation, novel formulations of Direct FE2 are proposed for heterogeneous problems in two situations where the scale separation is not fully satisfied. The first one is a static analysis. Instead of the classical Cauchy continuum, a micromorphic continuum is employed at the macroscale [2]. Besides the first-order displacement gradient, nonlocal kinematic fields are introduced and therefore a higher-order deformation mode at the microscale is modelled. The second one is a transient analysis. While a stationary micro-scale problem is normally assumed in the classical method, micro-inertia is considered herein [3, 4] and its importance is highlighted, especially the inertia contributed by the inclusions. It is shown that the implementation with Direct FE2 remains simple albeit the complicated microscopic responses. Finally, the proposed formulations are verified through several numerical examples, in which interesting physics phenomena are captured including size effects and wave mitigation.

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Fatigue Strength Simulation of Discontinuous Fiber CFRP Considering Viscoelastic-Viscoplastic Entropic Damage

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Key Words: *CFRP, Cyclic Loading, Numerical Analysis*

In order to evaluate the durability of CFRP, it is necessary to understand the damage and fracture behavior of the resin part. In order to evaluate the durability of CFRP, it is necessary to understand the damage and fracture behavior of the resin part. Conventional studies on the damage and fracture behavior of base resin have been limited to discussions under specific conditions[1,2]. However, in order to essentially discuss durability, it is necessary to establish a constitutive law for the resin that can evaluate the residual strength after experiencing various loading histories. With regard to the damage criterion, recent attempts have been made to clarify the damage evolution of materials based on irreversible thermodynamics. It is known that the thermodynamic entropy increases with the deformation of a material and fracture occurs when it reaches a certain value[3]. Therefore, it is expected that the irreversible entropy in materials can be a criterion to evaluate the damage of materials. In recent years, CFRP is required to have a design life of several decades depending on the field, and fatigue strength as well as static strength is becoming more important to ensure safety.. The purpose of this study is to predict the effect of fatigue on the base resin PA6 of CFRP as the first step of the long-term fatigue analysis of CFRP considering the nonlinear viscoelastic-viscoplastic constitutive law with entropy damage and the temperature and time dependence of the base resin. In this study, we first coded a viscoelastic-viscoplastic model that considers the damage caused by energy dissipation. Here, the damage is calculated from the energy dissipation due to the deformation of the dashpot, and when the damage reaches 25% (i.e., 25% voids), the elastic modulus is reduced to the original 1% because the resin becomes almost non-functional, and the stress of the previous increment is also calculated sequentially according to the updated elastic modulus. Then, uniaxial cyclic loading simulations were performed on a simplified model of discontinuous fiber CFRP, which was adapted from the viscoelastic-viscoplastic model presented earlier. The proposed viscoelastic-viscoplastic model was applied to a simplified model of discontinuous fiber CFRP, and uniaxial cyclic loading simulations were performed with a strain amplitude of 3.0×10-2, 30 cycles of tension and compression, and a strain frequency of 0.2 Hz. As a result, stress relaxation due to viscoelasticity was observed up to about 60 seconds, and after that, stress decreased as the number of damaged and destroyed resin elements increased. In this study, the proposed viscoelastic-viscoplastic model was applied to a simple model of discontinuous fiber CFRP, and uniaxial cyclic loading simulation was performed. As a result, stress relaxation due to viscoelasticity and stress reduction due to damage fracture of the resin were shown. The results showed that the stress relaxation by viscoelasticity and the stress reduction by resin damage and fracture were observed. For the long-term fatigue analysis of CFRP, it is necessary to simulate the cyclic loading with a model closer to the reality, and to compare the results with the experimental data and fitting.

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Finite Element Analysis for Failure Prediction of CFRP Cross-Ply Laminates Considering Viscoelastic Model with Entropy Damage

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Key Words: *FEA, Viscoelasticity, Thermodynamic Entropy, Damage Mechanics, Failure Prediction*

The long-term durability of viscoelastic materials is very important for discussing the durability of polymer composite materials. The polymer materials used for matrix of composite have time and temperature dependent characteristic which called viscoelasticity. In order to describe the material behavior accurately, a time- and temperature- dependent constitutive equation considering material damage is required. In this study, we propose a viscoelastic constitutive equation for viscoelastic media based on irreversible thermodynamics and viscoelastic theory [1] in order to predict failure behavior of heat-resistant carbon fiber reinforced plastics (CFRP). Regarding the material damage law, we introduce a thermodynamic entropy to material damage. It has been attempted to clarify the damage evolution in solid materials from irreversible thermodynamics in recent years [2]. Inelastic deformation of the material causes an irreversible structural change inside the material. Such an internal structural change is expressed by a thermodynamic internal variable based on Clausius-Duhem inequality (the second law of thermodynamics); i.e., deterioration of the material proceeds with the disorder of the system. The disorder in the system, which causes deterioration of the characteristics, is raised by the mechanical deformation and the entropy increases accordingly. The disorder in the degraded system continues to increase to the critical state and causes the failure of the materials. Therefore, irreversible entropy in materials can be used as a criterion for evaluating durability of materials. Single axis tensile tests are performed under various temperature and strain rates to determine the material properties and the amount of entropy generation. Furthermore, we introduced presented constitutive equation into representative volume element (RVE) model in order to predict the initial cracking under fatigue condition. Fatigue tests for cross-ply laminates are conducted to verify presented model.

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Identification of disbond and delamination in a honeycomb sandwich structure using air-coupled guided wave ultrasonics

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Key Words: *Hidden defect, Air-coupled ultrasound, CFRP, Honeycomb, Sandwich structure*

CFRP sandwich composites are finding increased use in various industries including aerospace and automotives due to many distinct advantages. However, they are highly susceptible to debonding and delamination damages especially under fatigue loadings or unexpected impacts during the manufacturing and in-service process. These damages could reduce the mechanical performance of the composite and thus pose serious problems for the safety and integrity of the whole structure. Guided wave (GW)-based inspection techniques are one of the potential solutions to detect such hidden defects in composite structures because GWs are able to propagate over a long distance and penetrate into internal laminates. Conventional GW-based inspection uses either immersion or contact transducers. This is frequently not practical, particularly under harsh environments or with large structures for field inspection. A non-contact inspection technique for delamination and disbond in a sandwich structure is demonstrated in this work using air-coupled ultrasonic guided waves. The sandwich plate used in this study comprises of a Nomex® honeycomb core embedded between two CFRP composite skins. The dispersion characteristics of the CFRP laminate and sandwich plate are investigated both in numerical simulation and experiment to validate the constructed numerical model of the sandwich structure. The inspection frequency, wave mode as well as incident angle of the air-coupled transducer can be determined by frequency-wavenumber analysis. Numerical simulations are further conducted to explore guided wave propagation mechanics due to delamination and disbond. Both the delamination and disbond can be detected in numerical simulation. A parametric study is carried out to optimize the configuration of air-coupled transducers in simulation. The set-up of transducers is subsequently applied in the experiment for the disbond identification. Tests have been carried out on honeycomb sandwich samples with disbond. The measurements are compared with numerical predictions and good agreement is obtained.

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Improved Numerical Simulation of Woven Textile Membranes using Stress-Ratio-Dependent Material Properties

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Key Words: Woven Textile Membranes, Nonlinear Material Modeling, Improved Structural Simulation

A newly proposed hyperelastic orthotropic material model [1] for the geometrically nonlinear simulation of woven tensile membranes is extended to become the basis of a new approach for structural simulations of higher accuracy. The model is polyconvex and benefits from anisotropic metric tensors in the formulation of structural tensors which enable various interactions and couplings between principal material directions [2]. The model contains only 3 stiffness-related material properties for glass-PTFE fabrics which makes it a competitive replacement of the commonly used linear elastic formulation.

To enhance the model response in numerical simulations a new framework is proposed to adjust and identify material properties based on the stress ratios appearing in structural problems. To this end, initially, the material parameters are separately adjusted to classical biaxial tensile tests with varying load ratios, e.g., 1:1, 0.5:1, etc., and additionally rather uncommon stress ratios 1:0.125, 1:0.75, etc. In a second step, an iterative simulation procedure will be applied, where, according to the locally obtained stress ratios within the discretized structural problem, the corresponding parameter values are updated at each integration point. The parameter values for stress ratios in between the experimentally measured ones are computed using a proper interpolation scheme. The iterative scheme is repeated until the overall parameter change on all points becomes negligible.

Aside from this approach, a more directly data-based procedure is proposed which already allows the description of the membrane's nonlinear response by still considering the linear-elastic model. For this, depending on the current local stress-ratio and stress intensity, a set of elastic constants of the linear elastic formulation is identified from a suitable interpolation scheme directly using the experimental data. Thereby, a continuously increasing cloud of computed material properties is used as the reference to update the locally varying stress-strain relation. Finally, both methods are compared with more classical approaches in realistic structural problems.

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Modelling of angle-ply Fiber-Reinforced Composite laminates with Direct FE^2

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Key Words: *Multi-scale, homogenization, composite, pipe, failure, fibre rotation*

Abstract

Direct FE^2 [1, 2, 3] is a computationally attractive [4] FE^2 implementation as both the macro and micro-scale can be run in a single finite element analysis. The method is versatile as the in-built constitutive material models in a commercial FE software can be deployed easily to model any behaviour of the material micro-structure constituents and can be implemented on any commercial FE software that supports Multi-Point Constraints.

The Direct FE^2 method, models composite laminates using micromechanical single ply Representative Volume Element (RVE) [5,6]. The non-linear shear and damage behaviour of angled ply laminates is studied and simulated with the Direct FE^2 approach. Angled ply laminates are focussed since their non-linear behaviour arises from matrix plasticity and fibre reorientation in addition to constituent damage. This bottom-up approach needs only constituent (matrix and reinforcement) properties as input, thus eliminating the requirement for time consuming and expensive laminate and ply-level mechanical properties characterization. Matrix micro-cracks and fibre fracture are simulated using cohesive zone models. The results of the angle ply laminate simulation are compared with experiments. The fibre rotation observed in the various Direct FE^2 laminate models is also compared with existing model predictions. The Direct FE^2 simulation capability of composite structures is demonstrated by applying the method to model an angle ply laminate composite pipe (subjected to tension, torsion and bending) [6] from the constituent level and compared with experiments.

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Moving Particle Simulation for Compression Molding of Polymer Matrix Composite Rib Considering Fiber Deformation

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Key Words: *Particle Method, Polymer Matrix Composites, Compression Molding, Bead-Chain Model*

Compression molding is suitable for producing complex-shaped polymer matrix composite components owing to its short cycle time and low costs. In the method, the mold cavity is charged with the molding material using the two-part mold system, and the component is produced by fluidizing the material using a press machine. The components made by compression molding are susceptible to the uneven distribution of the resin and fibers. It is easy to occur short shots in the rib structure when producing the structure by compression molding. The strength and stiffness of the components are highly affected by the fiber distributions. To control the mechanical property of the molded components, it is essential to understand the various phenomena in the molding process.

The distribution of fiber orientations is affected by the molding process. Therefore, the multiphase flow analysis of fibers and resin is needed to understand the whole process of compression molding. Moving particle simulation (MPS) is suitable to explicitly model the fibers and resin using particles. The fiber orientation distribution and resin rich areas in injection molding of short-fiber-reinforced composites were predicted using the MPS method [1,2]. However, these previous studies assumed that the fibers are rigid. The elastic fibers that can be stretched and bent are required in compression molding of the rib structure because the fibers should be deformed at the entry and the tip of the rib.

This study develops the three-dimensional multiphase flow analysis considering the resin flow and the elastic fiber deformation. MPS is used to explicitly model the resin and fibers. The simplified bead chain model proposed by Sasayama et al. [3] is adopted to consider the fiber stretching and bending deformations. To verify the proposed analysis, the three-dimensional compression molding analysis of the cross-ply composite rib structure is conducted. The numerical results showed that the fibers bent when flowing into the rib and that the ply structure was maintained. These predicted phenomena qualitatively agreed with the experiments [2].

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Multiscale analysis for prediction of process-induced warpage on asymmetric CFRP laminate

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Key Words: *CFRP, Process-induced deformation, Multiscale analysis, Molecular dynamics, Finite-element analysis, quantum-chemical reaction path,*

Four-scale analysis composed of a quantum-chemical reaction path calculation, a curing molecular dynamics (MD) simulation[1, 2], a microscopic finite-element analysis (FEA), and a macroscopic FEA was developed to predict manufacturing process-induced deformation of composite laminate.
In this approach, thermomechanical properties, volumetric shrinkage due to curing reaction, and gelation point of matrix thermoset resin were predicted first by using MD simulations coupled with quantum calculations. Orthotropic material properties and cure-shrinkage deformation of unidirectional laminae were then evaluated by periodic unit-cell (PUC) analysis [3] using microscopic FEA based on the values obtained in the MD simulations. Finally, process-induced deformation of asymmetric cross-ply laminate due to cure and thermal shrinkage was predicted by macroscopic FEA analysis in which each layer of the laminate was modeled as an orthotropic homogeneous body by homogenization in PUC analysis. The predicted warpage of asymmetric laminates by using the presented multiscale analysis and experiments were in good agreement. In addition, the effects of the matrix resin species on the macroscopic deformation behavior were explored from the viewpoint of molecular scale using this multiscale analysis.
The results presented here provide important knowledge for the development of high-performance composite parts and stable manufacturing.

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Multiscale failure analysis of flame-retardant CFRP laminates

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Key Words: *CFRPs, Open-hole tensile/compressive tests, Finite element analysis*

Stress concentrations around small holes (for fasteners) in carbon fiber reinforced plastics (CFRPs) have been studied for decades, especially in aerospace. Open-hole tensile (OHT) and compression (OHC) strength is a determining factor in the design of composite structures. The hole triggers stress concentrations and inherently reduces the net section volume. OHT and OHC testing is a prerequisite to leverage the use of composites in load-bearing structural applications. In the design of aircraft structural components using composite materials, it is necessary to verify all the factors that directly affect the strength (such as stress concentrations around holes as mentioned above), but due to the diversification of types of damage and failure due to the complexity of the structure, attempting to verify all of these by testing results in a significant increase in development costs and a longer development period [1]. For these reasons, in recent years, virtual testing has been attracting attention, which attempts to replace the certification test of CFRP laminates with numerical simulation [2]. Here, we forcused on the advanced CFRP laminates such as flame-retardant thermoset CFRP and investigated the stress-strain response of the OHT and OHC specimens. Furthermore, mesoscale fracture behavior of CFRPs are discussed by a finite element analysis.

In recent years, the eXtended Finite Element Method (XFEM), which can model cracks independently of the mesh, has been proposed and is applied to the damage progression analysis of CFRPs. In this study, mesoscale failure analysis of open-hole laminates is carried out for CFRPs. Matrix cracks in the layers and delamination between layers are the main damage mechanism, so XFEM is used to model matrix cracks independently of the mesh, and delamination is modeled by inserting interface elements between layers. The parameters for the XFEM model were determined based on the experimental results for uniaxial tensle/compressive tests and in-plane shear tests. Then, the prediction accuracy of the presented method is verified by predicting the progressive damage and strength, and comparing it with the experimental results of OHT and OHC tests. The effects of the matrix properteis on the transverdal tensile/compressive strangth and shear strength were also discussed by periodic unit-cell analysis.

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Multiscale Modelling of Fiber Reinforced Composite Beams with Shear-Flexible Beam Elements using Direct FE^2

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Key Words: *Multiscale Modelling, Fiber Reinforced Composites, Shear-Flexible Beam Elements, Direct FE^2, Multi-Point Constraints*

Modelling fiber reinforced composites with high fidelity finite element (FE) analyses has always been challenging due to the large separation of length scales between a composite part and its constituent details. Current available computational resources put a limitation on the amount of details that can be modelled simultaneously. This means that important microscale mechanics such as fiber-matrix interactions may not be adequately captured when fiber reinforced composites are modelled at the part level or even at the ply level.

Multiscale modelling methods present an opportunity to marry these analyses across different scales by utilising the separation of length scales. Multiple analyses at different scales can be performed on the same problem to provide a more accurate prediction, while scale transition relationships are enforced between them such that the analyses remain consistent.

Here, a multiscale homogenisation model for fiber reinforced composite beams that is based on the novel Direct FE^2 framework will be presented [1]. At the part scale (macroscale), the computational efficiency of shear-flexible beam elements will be tapped upon. Its constitutive responses are provided by concurrent microscale analyses performed using explicitly modelled representative volume elements (RVE) of the composite. This reduces the computational cost to a fraction of that required in a true high fidelity analysis, making it much more feasible.

Scale transition relationships are enforced using multi-point constraints, which are readily available in most FE software. Kinematic downscaling of the macroscale loads is done by imposing appropriate periodic boundary conditions onto the RVE. On top of this, a separate constraint is required to impose the RVE shear angle, which has been successfully achieved via a weighted integral constraint. Kinetic upscaling of the microscale responses is done by appropriately scaling the RVE mesh volume. The scaling factor is governed by the Hill-Mandel homogenisation condition and Gaussian quadrature, and is imposed such that the strain energies across all the RVEs sum up to the corresponding macroscale value they represent.

In contrast to the more well known classical FE^2 approaches, Direct FE^2 offer a much simpler implementation for this multiscale framework. A generic, transferrable Python script is used to set up the model, presenting the opportunity for even users less experienced in multiscale modelling to utilise it. Beyond composites, the framework can be applied to a wide range of problems, as long as the base materials are known and an appropriate RVE can be constructed. Furthermore, this framework can be readily expanded to plate elements for flat composite structures as well.

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Multiscale-Multiphysics Simulation of Process-Dependent Mechanical Properties of Thermoplastic Composites

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Key Words: *Homogenization method, Phase-field method, CFRTP, Crystallization*

In recent years, the application of carbon fiber reinforced thermoplastics (CFRTPs) in aircraft structures has been broadening. Although they are mainly applied to the secondary structural components so far, they are expected to be applied to the primary structure in near future. The advantages of CFRTPs are their short manufacturing time, weldability, and recyclability. However, it is well known that their structural performance significantly depends on the manufacturing condition because the morphology of thermoplastic polymer is developed depending on the manufacturing (solidification) process. So far, many experimental studies have been performed on the cooling-rate dependent morphology and resultant mechanical properties of thermoplastics [1-3]. However, to the best of authors' knowledge, there is no numerical model and simulation scheme which is able to predict the performance of structural components made of CFRTPs from their manufacturing condition.

The objective of this study is to establish a numerical scheme to predict the structural performance of CFRTP components based on the manufacturing condition. The proposed scheme consists of two simulations; phase-field simulation and homogenization simulation. Firstly, the phase-field simulation [4-6] is performed to predict the morphology development (i.e., crystallization) of thermoplastics based on the solidification condition. Then, the homogenization simulation on the predicted morphology is carried out to predict the mechanical properties of CFRTP. The proposed scheme is verified against the experimental degree of crystallinity, rate of crystallization, and the resultant mechanical properties.

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Nonlinear Buckling, Post-buckling and Collapse of Composite Thin-walled Lenticular Tubes Subjected to Pure Bending

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Key Words: *Nonlinear buckling, post-buckling, collapse, thin-walled structures, finite elements*

The composite thin-walled lenticular tubes (CTLTs) have been proposed as one of the most promising candidates for solutions of various light-weight large-scale deployable structures such as solar sails and wrapped-rib antennas in space[1]. Since the thin-walled tubes or booms are thin in thickness and have long aspect ratio, structural instability arises as one the biggest concerns for structural designs. This paper presents some numerical investigations on the nonlinear buckling, post-buckling and collapse behavior of the CTLTs subjected to pure bending[2]. First, an automatic implicit finite element (FE) simulation scheme accounting for high geometric nonlinearity was proposed for accurately predicting the nonlinear critical buckling load and the corresponding nonlinear buckling modes, as well as the postbuckling response of CTLTs. Next, an explicit dynamic finite element procedure was developed to analyze the quasi-static bending collapse of CTLTs. The effect of cross-section shapes on the performance (i.e., bending stiffness, nonlinear critical buckling load, and collapsing load) of CTLTs was highlighted through a parametric study performed on a variety of geometric configurations with the same weight but different cross-section shapes. The outcome of this work would enhance the understanding of nonlinear buckling, post-buckling, and collapse behavior of CTLTs, and open the door for cross-section shape design of CTLT structures.

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Numerical Simulation of Temperature Elevation during Ultrasonic Welding Process of CFRP

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Key Words: *Ultrasonic welding, Numerical simulation, CFRP.*

Carbon fiber reinforced plastics are widely used in the aerospace industry because of their superior specific strength and stiffness. Although thermoset composites have been mainly used in the past, thermoplastic composites have been attracting attention in recent years from the viewpoints of moldability and productivity. Thermoplastic composites have excellent impact resistance, recyclability, and short processing time. In addition, the characteristics of thermoplastic resin can be utilized for welded joints. By assembling components without using bolts or rivets, it is possible to reduce weight and stress concentration. One type of welding is ultrasonic welding. Ultrasonic welding is a method of welding by melting resin using the heat generated by transmitting vibration energy to the welding interface, and it can be done in a short time at normal temperature and pressure with energy saving[1]. However, the process parameters such as welding pressure, welding time, amplitude, and frequency are intricately related, and it is difficult to predict the optimum setting of these parameters, so the method has not yet been generally applied[2].

In this study, the temperature rise during the ultrasonic welding process was simulated and compared with the results measured experimentally. In the simulation of ultrasonic welding, the ultrasonic vibration is on the scale of 10^{-5} s, while the welding time is on the scale of 10^{0} s. The difference in the time scales causes a long calculation time. In this paper, we propose a multi-time-scale simulation method that can simulate the weld process with high accuracy and short calculation time. In the multi-time-scale simulation, the temperature rise per microsecond at each initial temperature of 25°C is calculated in the microsecond-scale simulation. Then, normal-scale simulation, in which the ultrasonic vibration is replaced by a constant load, is used to simulate the entire ultrasonic welding process accurately by fitting the microsecond-scale simulation with the material properties as variables. In the ultrasonic welding process, a neat polymer protrusion called an energy director (ED) is inserted between the materials to be welded. The ED acts as a starter for softening and melting of the resin, and enables stable welding. Focusing on the ED, we investigated the effect of the shape on the temperature rise. The results of the study showed that the slope of the temperature rise was close to the simulation results obtained by multi-time-scale simulation. The energy dissipation due to viscoelasticity was found to be important in the temperature spike. It is also shown that the temperature spike is caused by stress concentration above a certain level.

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Self-deployment characteristics of CFRP bistable open sectional semi-cylindrical beam

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Key Words: *Self-deployment, Finite Element Analysis, Experiment, Plain Weave Composite, Strain Energy Distribution, Transitional Configuration*

Various deployable booms have been developed because simplicity, light weight and high storage efficiency are required for space deployment structures. One of them is an open sectional boom which is made of Carbon Fiber Reinforced Plastic (CFRP) plain weave composite molded into a cylindrical beam shape. This boom has a characteristic of having two different stable states, showing bistability. In the deployed state and the coiled (stored) state, it retains each shape without any external force or constraint. Once the triggering deformation is imposed to the coiled state, this boom autonomously transforms to the initial cylindrical beam shape.

It is observed that the deployment of the bistable beam may come to halt in the transitional state, and detailed analyses of the mechanism are required. Although Brinkmeyer et al. [1] introduced and considered the deployment force, it was evaluated without identifying various factors such as friction or air resistance. In addition, the decrease of the deployment velocity is investigated only on experimental basis, whereas the finite element analyses focus on the shape and deformation during the deployment in detail.

In this study, a series of the transitional configuration from the coiled shape to the deployed shape was simulated by finite element analysis. Rectangular plate specimen was used to directly measure the stiffness matrices (ABD matrices) that are used in the FE analysis. In order to consider the heterogeneity of fiber bundle in the plain woven fabric composite, the in-plane stiffness (A matrix) was obtained from the tensile test, and the out-of-plane stiffness (D matrix) was calculated from the result of the bending test and the torsion test. In the coiled state, the distribution of strain and curvature is generated in the cylindrical axis direction under the influence of the free edge. With reference to Fujioka et al. [2], self-deployment force is defined as the reaction force generated when a fixed rigid wall prevents the bistable beam from self-deploying. In addition, for each deployed length, the strain energy of whole bistable beam was calculated. It is found that the rate of change of strain energy with respect to the deployed length is equal to the reaction force of the rigid wall. To evaluate the validity of finite element analysis, experimental investigation is conducted and the self-deployment force were measured with the same method. The finite element analysis and experiment results show that the self-deployment force gradually increases as the bistable beam deploys, and converges to a constant value after a certain deployed length. The critical deployed length can be estimated from the strain energy distribution in the longitudinal direction.

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Steady-State Creep Analysis of Composite Spherical Vessels Using the Finite-Strain Theory

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Keywords: Composites, Spherical Vessels, Steady-State Creep, Finite-Strain Theory

ABSTRACT

The paper presents the steady- state creep analysis of spherical vessels of particulate composite materials using the logarithmic strain (finite-strain) theory. The paper develops (in an almost closed form) expressions for the stress and strain distributions in the spherical vessels. The stress and strain distributions are evaluated numerically at various radii of the spherical vessel and the results are displayed graphically. The effects of the particulate size on the stress and strain distribution are studied for several different particulate sizes and the results are exhibited graphically. Finally, the results from the present investigations are compared with the results for a spherical vessel of monolithic materials and the differences in the stress and strain distributions in the two types of the spherical vessels are clearly brought out. It is believed that the results from this research will aid the designers in selecting a spherical vessel of a material that will be most useful in meeting their requirements.

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Stochastic Stress Analysis of Unidirectional FRP Considering Random Fiber Location Variation in case of Higher Vf by Improved Mesh Superposition Method

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Key Words: *Stochastic Stress Analysis, FRP, Random Fiber Location Variation, Improved Mesh Superposition Method, Monte Calro Simulation.*

Composite materials have been widely used in various fields. Composites have superior mechanical properties such as specific rigidity or specific strength, but mechanical responses of composite structures have larger dispersions comparing to conventional homogeneous materials. In particular, a lot of stress concentrations due to non-homogeneous and not-perfectly controlled microstructure will be observed, and therefore stress analysis considering its inhomogeneity and a stochastic analysis considering microscopic random variations have been attracted [1]. In using finite element method for the analysis, one of the problems is difficulty when considering geometric randomness such as random fiber arrangement in fiber reinforced plastics (FRP).

For this problem, the Mesh Superposition Method[2] is attempted to be employed for the analysis, since the numerical model for the analysis can be easily generated even for materials with complex internal structures. In this research, an improved mesh superposition method-based analysis approach is developed for stabilizing the analysis of composites[3] based on the M^3 Method[4], and it is applied to stochastic stress analysis of unidirectional FRP considering random variations of fiber location. In the previous report[3], effectiveness of the presented approach is validated when fiber volume fraction (Vf) was assumed to be relatively low, and the relatively small location variation was considered.

In this report, for more realistic composites, the stochastic stress analysis of FRP with high Vf and large variation using the improved mesh superposition method is attempted, and the effectiveness and problems in the analysis will be discussed with some numerical examples.

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Strength estimation of composite material by peridynamics and in-situ observation

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Key Words: *Peridynamics, Composites, Fracture analysis, In-situ observation, Strength*

In this presentation, stress analysis of a unidirectional fiber reinforced composite material by coupling peridynamics and in-situ observation is discussed for apparent strength estimation of the material. Composite materials have complex microstructures and complex damage propagation caused by multiple cracks originating from the interface between the reinforcement material and the base material. For this analysis, for example, XFEM based approach or analysis using the cohesive element has been attempted, but the complexity and difficulty of these approaches, further effort for more efficient approach to analysis is needed. Furthermore, the apparent strength of the composite material varies due to the randomness / uncertainty of the microstructure. Therefore, in-situ observation is important for the accurate representation of the real material model and from the viewpoint of Verification & Validation. From this background, we attempted to employ the peridynamics method [1] to the stress analysis of composites and in-situ observation using a digital microscope. In this method, the formulation is based on integral equations and the target object is spatially discretized by particles, and it will be more effective for modelling and solving problems involving many inclusions and discontinuities such as cracks than conventionally used analytical methods such as finite element method. For the in-situ observation, the status of an actual composite specimen during tensile testing is accurately observed using a digital microscope [2].

Firstly, outline of the problem setting, peridynamics and in-situ observation are explained. Some numerical results on the stress analysis of the fiber reinforced composite plate under transverse tensile load by in-situ observation-aided peridynamics analysis are shown. Validity and effectiveness of the analysis based on the coupling of peridynamics and in-situ observation for composite material are investigated, and applicability of the method to the analysis of a fiber reinforced composite material is discussed.

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Structural Evaluation in Lattice-Based Mechanical Metamaterials Fabricated by AM for Lightweight Tunable Structures

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Key Words: *Structural Analysis, Multiscale Analysis, Lattice Structures, Mechanical Metamaterials*

Mechanical metamaterials are artificially manufactured materials with properties, which cannot be obtained from natural materials, consisting of deliberately designed microscopic internal structures [1]. Those conceptual artificial materials are ready to fabricate with the advent of the additive manufacturing technology. Recently, a class of metamaterials has been actively studied due to its potentials for performance improvements and extensions of structural capabilities. Mechanical metamaterials can exhibit exotic material characteristics and/or macroscopic behaviors attributed to their micro/mesoscale internal structural designs such as truss or porous in μm/mm order in addition to material properties constructing the structural components. For example, metamaterials having unique properties such as zero Poisson's ratio, ultralight weight less than 0.01 g/cm^3, simultaneous lightweight and high stiffness (approximately 700 kg/m^3 and 1 GPa) are hoped to realize high-performance structures [2].

In this paper, structural characteristics of lattice-based mechanical metamaterials will be studied. The objectives of this paper will be 1) to develop an analysis framework, which enables structural evaluations to design mechanical metamaterials, 2) to demonstrate the feasibility of the methodology to evaluate structural characteristics of lattice-based mechanical metamaterials, and 3) to explore and study the potential and structural integrity of lattice-based mechanical metamaterials.

In order to efficiently model such structures, a computational homogenization method for lattice-based mechanical metamaterials capturing characteristics of a representative unit cell is implemented. A unit cell of the periodically distributed structure is modelled as representative finite elements, and the equivalent stiffness properties of the unit cell are calculated based on the computational homogenization procedure. The obtained equivalent stiffness properties are used to perform a multi-scale structural analysis of lattice-based mechanical metamaterials. Similarly, stress amplification factors recovering a stress distribution in a microlattice structure based on a macroscopic stress distribution, which is obtained from the multi-scale structural analysis, will be calculated with the present finite element procedure. A microscopic stress distribution recovered based on stress amplification factors will then be used for strength evaluation.

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Temperature Response of CFRP Exposed to Simulated Lightning Current

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Key Words: *CFRP, Lightning strike, Multiphysics Problems, Industrial Applications*

Carbon fiber reinforced plastic composites (CFRP) have been applied to primary structures of aircrafts with the aim of improving fuel efficiency because of its mechanical property. Aircrafts are sometimes struck by lightning in flight, resulting in damage of structures. Once the surfaces of CFRP structures are damaged, inspection and repair are required. To reduce the lightning strike damage, it is important to clarify the damage mechanisms caused by lightning strike. Lightning strike damage are caused by complex physical and chemical phenomena such as Joule heat generation, thermal decomposition of matrix resin, breakdown, combustion, acoustic force, electro-magnetic force and others. Because of the complexity of the phenomena, the effects of each phenomenon on lighting damage are not understood in detail. Objective of this study is to understand the effect of Joule heat generation on lightning strike damage with lightning current test. The static and impulse lightning current was directly applied to CFRP specimen by performing conduction tests to avoid the effect of arc root behavior and acoustic force. Temperature response was measured by using a thermal camera. Finite element analysis was conducted to estimate joule heating effect caused by lightning current.

CFRP laminates were fabricated from unidirectional carbon fiber/toughed epoxy prepreg tapes (IMS60/133, Toho Tenax Co. Ltd., Japan). The stacking sequence were $[0]_{16}$ (16 plies). A specimen had 10 mm width, 50 mm length and 2.2 mm thickness. Lightning current was applied with an impulse current generator (Haefely Hipotronics). Component A waveform in accordance with SAE ARP 5412B was applied to an electrode which was connected directly to edge of specimen. The other electrode, which was directly connected to edge of specimen, was connected to ground. The maximum current peak value was 10 and 20 kA. Lightning strike phenomena were captured by using a high-speed camera (Shimadzu Corp.) and a thermal camera (FLIR Systems, Inc.). As results, pyrolysis gas at the side surface was observed immediately after the current injection. Changing temperature distribution state over time was successfully obtained by a thermal camera. Temperature response estimated by finite element analysis showed good agreement with experimentally obtained results.

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The Mechanical Response and Failure Mechanisms of Natural Fiber Reinforced Composite Laminates: A Computational Study Validated by Experiments

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Key Words: *Natural Fibers, Anisotropy, Unidirectional Composite, Numerical Analysis*

Concerns about the environmental situation, namely pollution and wasteful use of fossil fuels, have generated a great demand for the development of new environmentally friendly materials for use in various fields. Natural fiber-reinforced composites are seen as a good alternative to traditional synthetic fiber composites. However, for natural fiber composites to be an adequate replacement, they must demonstrate sufficient mechanical strength, especially for load-bearing engineering components or structures. This study investigated the strength of materials composed of unidirectional sisal fibers (grown in the Negev region of Israel) within a thermosetting polymer matrix, containing 20%, 40% and 60% fiber volume fraction. Experiments in conjunction with finite element modeling were utilized to determine the effective mechanical response and failure modes of the composite for the different material compositions. Tensile tests on the composites were performed with loading along the fiber and at an angle of 45° to the fiber direction. Tensile testing along the fiber direction was also carried out on specimens with holes and notches for various fiber volume fractions. Assuming the unidirectional composite behaves as a transversely isotropic material [1] with an anisotropic fiber, both analytical [2] and micro-mechanical numerical models were used to estimate the effective mechanical properties as a function of the sisal volume fraction, and a comparison was made with the experimental results. A macroscopic approach was used to simulate the tensile tests. During the simulation, the parameters of the damage evolution were determined, and the parameters of damage initiation were validated. Finite element analysis was carried out using Abaqus™ software. The study shows that the behavior of sisal fiber reinforced composites is linear elastic prior to failure. The average longitudinal modulus of elasticity of the sisal fibers is 25 GPa, the average tensile strength of the fibers is 490 MPa with a strain at failure of 1.5-2%. The fiber transverse modulus of elasticity determined by finite element analysis is 1.6 GPa. It was observed that failure form depends on the volume fraction of the fibers; in materials containing a smaller amount of fiber, a localized failure band perpendicular to the direction of the fibers occurs, while for materials containing a greater amount of fiber, failure in the form of splitting along the fibers takes place. The results of this study shows that materials with sisal fibers can reach tensile strength of 250 MPa, which are comparable to high strength aluminium and thus can be used in structural applications. The simulation results are in good agreement with the experiments.

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Three-dimensional Stress Fields in Tapered Laminated Composites with Internal Ply Drops

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Key Words: Tapered composites, ply drops, localised 3D stresses, Unified formulation

Wind turbine blades often vary in thickness throughout to optimize local strength and stiffness. Changes in thickness of laminated composite structures results in ply drops, where the number of through-thickness plies of a composite structure suddenly changes. Ply drops represent sudden changes in not just geometry but also material properties. Both can cause stress concentrations leading to structural failure [1]. In order to minimise the effect of local stress concentrations, they should not be positioned in stressed areas.

Although closed-form solutions exist for the stress state in ply drops, they do not replicate the complex non-linear behaviour and the interactions between ply drops. Current work uses a novel variable kinematics continuum finite element to model the tapered laminate structure with high accuracy. Based on the Unified Formulation (UF), the element uses a hierarchical, Serendipity-Lagrange expansion based model to describe the kinematic field.

Previous work using this element considered prismatic structures solely consisting of hexahedron shapes. Modelling composite structures with a layer-wise approach has shown high accuracy using this approach [2]. However, modelling ply drops requires using other elements, such as wedge elements. Modelling non-hexahedron geometries is achieved by collapsing nodes, similar to degeneration of element formulations in conventional finite element analysis.

Tapered composite panels featuring multiple ply drops are analyzed. The results will include direct comparisons between the formulation and conventional finite element models. Early work has already shown excellent agreement in the stress fields with a significant ($\sim$ 4x) reduction of the degrees of freedom.

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An Anisotropic Damage Model for Prediction of Ductile Fracture during Cold Forging

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Key Words: *Ductile fracture prediction, cold forging, finite element analysis, anisotropic damage*

Researchers have formulated equations of ductile fracture to simulate and predict defects in cold-forged parts, e.g., the Cockcroft–Latham criterion [1]. However, these equations are not applicable to certain cases of fracture in forged products. This study formulates a new equation for predicting ductile fractures with better prediction accuracy than the convention by which cost for trial-and-error design can be reduced.

The equation is expressed as a second-rank symmetric tensor, which is the inner product of the stress and strain-increment tensors. The theoretical efficacy of the equation in predicting ductile fractures is verified via a uniaxial tensile test.

The practicability of the equation is confirmed by applying it to the simulations of two real cold-forged components: a cold-forged hollow shaft and a flanged shaft. For the hollow shaft, the equation predicts the position where the ductile fracture would initiate, which—to the best of the authors' knowledge—is unique to this study. For the flanged shaft, the equation predicts the occurrence of diagonal cracks due to different lubrication conditions.

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Investigating the influence of material ductility on the failure prediction capabilities of the continuum damage mechanics approach: A computational study validated by experiments

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Key Words: *CDM, Ductile failure, FEA*

In order to properly characterize failure limits for metallic materials, the scientific community has developed numerous failure criteria. These criteria can in general be classified into two different categories: criteria that differentiate between damage initiation and damage evolution, and criteria that do not. Currently, there is no agreement in the scientific community regarding the most accurate criterion when it comes to predicting damage initiation and/or evolution. Many of the ductile failure criteria incorporate some triaxiality dependent plastic strain measure as a governing parameter for ductile failure initiation. Nevertheless, to the best of the authors' knowledge, a study, dedicated to investigating the accuracy of different criteria on the specific ductility of a material has not been conducted. It could be that a certain criteria are valid only for limited values of ductility.

In this study, experiments in conjunction with computational analyses were conducted in order to investigate the influence of the materials ductility on the failure prediction capabilities of different failure criteria based on the Continuum Damage Mechanics (CDM) approach. Two different aluminum alloys with different levels of ductility were selected Al7075-T651 and Al2024-T351. Compression experiments on three different specimen geometries were conducted. The displacement and strain fields were measured using Digital Image Correlation (DIC). Each specimen geometry resulted in a unique triaxiality-plastic strain relation up to initial failure. Finite element models of the experiments were developed and used to study the deformation process upto and including failure. The models underwent a standard solution verification process and validation against the DIC and the force-displacement measurements. The computations were used to quantify the different parameters required in order to determine failure initiation and evolution for the various criteria examined (stress, strain and energy density based criteria). The computational-experimental methodology reported in [1] and based on [2] was used to generate a damage initiation failure curve for each alloy. An energy based damage evolution criterion was implemented in order to model damage evolution and crack propagation. Finally, three point bending experiments on bars with complex geometries were conducted in order to test the different criteria against data which was not used in the initial parameter identification process.

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Numerical Simulation of Ductile Fracture Based on A Novel Damage Evolution Model

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Key Words: *Numerical Method of Ductile Fracture, Damage Evolution, Damage Level Definition, Void Shape Effect*

Numerical simulation has increasingly become an extremely significant tool to predict ductile fracture and is of great significance for engineering application. Ductile fracture includes void nucleation, growth and coalescence at micro level. Therefore, a reliable damage model based on void evolution is an effective part of numerical method to investigate ductile fracture.

A novel damage level was given and defined as the ratio of the maximum statistical cross-sectional area of voids to the cross-sectional area of the representative elements. Void nucleation is continuous in the whole deformation process [1], which was described by statistical theory in our investigation. Under arbitrary load condition, void growth includes not only volume change but also shape change [2]. Combined with the void number continuous equation, a novel damage evolution model including void nucleation, volume change and shape change was derived. Based on the proposed damage evolution model, a series of numerical simulations were conducted on tensile fracture of aluminum specimens under different loading state. The effects of specimen shapes on stress state, strain state and void number distribution were summarized by numerical simulations. The corresponding numerical predictions were verified by the experimental results under the same load and a good agreement was obtained between numerical and experimental results. The consistency of comparison clarifies that the presented novel damage evolution model is reliable.

The numerical predictions include both shear fracture and tensile fracture with different levels of stress concentration. All predictions agree well with experiments both from macroscopic fracture morphology and microscopic void distribution of the fracture. The parameters involved in this model can be directly obtained by experiments and it made the application of this model simple. Such definition of damage level in our model has clear physical meaning and requires no additional critical damage level to characterize failure. The numerical simulation with such damage model is a powerful numerical method to analyze ductile fracture under different stress states. Such numerical method provides a convincible theoretical support for engineering design.

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Predicting Ductile Fracture during Sheet Stretching by a Modified Miyauchi Test Using an Ellipsoidal Void Model

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Key Words: *Ductile Fracture, Void Model, Sheet Stretching, Miyauchi Test, Prestrain*

Ductile fracture is a microscopic phenomenon because it occurs through nucleation, growth, and coalescence of voids. Since the ductile fracture criteria that are widely used for metal-forming processes, such as those introduced by Cockcroft and Latham, Brozzo et al., and Oyane, are derived from a macroscopic viewpoint, it is challenging to improve the prediction accuracy for a microscopic ductile fracture phenomenon using a macroscopic ductile fracture criterion. Although nucleation and growth of voids are simulated in the Gurson model, the coalescence of voids cannot be simulated intrinsically. Hence, for instance, the coalescence of voids is assumed to occur when the void volume fraction reaches a critical value. However, this assumption is inappropriate, because the critical void volume fraction depends on the stress state. Hence, the coalescence of voids should be evaluated using a model with a definite physical meaning.

The author has attempted to predict ductile fracture during metal-forming processes from a microscopic viewpoint [1]. The author's proposed model of void coalescence is based on the two-dimensional void model proposed by Thomason and that proposed by Melander and Ståhlberg, which are also derived from a microscopic viewpoint. Both the Thomason model and the Melander and Ståhlberg model assume that the void is rectangular and that the direction of the major axis of the void coincides with the direction of the maximum principal stress. In contrast, the author's proposed model assumes that the void is ellipsoidal and that the direction of the major axis of the void does not coincide with the direction of the maximum principal stress. Hence, the author's void model can be used for simulating metal-forming processes.

In this study, an ellipsoidal void model [1], which has been proposed by the author, is evaluated by the sheet stretching using a modified Miyauchi test [2], which was originally proposed to evaluate the relationship between the shear stress and the shear strain. A number of experimental researches on the prediction of ductile fracture during the sheet stretching have been performed. However, few researches on the effect of prestrain on ductile fracture have been performed. Hence, in this study, the effect of prestrain, which is applied to a sheet by rolling, on ductile fracture during the sheet stretching, has been clarified numerically and experimentally.

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Accurate absorbing boundary conditions for two-dimensional peridynamics

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Keywords: Two-dimensional peridynamics equation of motion; absorbing boundary condition; corner reflection.

The aim of this paper is to construct accurate absorbing boundary conditions (ABCs) for the two-dimensional peridynamics equation of motion which describes nonlocal phenomena arising in continuum mechanics based on integrodifferential equations. To this end, a full discretization of the system is used based on a Crank-Nicolson scheme in time and an asymptotically compatible scheme in space. Recursive relations for the Green's functions are then derived and numerically used to evaluate the nonlocal ABCs. In particular, these absorbing boundary conditions solve the corner reflection problem with high precision. The stability of the complete fully discretized scheme is stated and numerical examples are finally reported to demonstrate the validity of the resulting ABCs.

Component-wise fracture analysis through coupled three-dimensional peridynamics and refined one-dimensional finite elements

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Key Words: *Carrera Unified Formulation, Peridynamics, Fracture, Multi-component structures*

Peridynamics (PD) is a non-local theory introduced by Silling in [1]. It is based on integro-differential equations, which means that PD could be employed for the investigation of problems with discontinuities, such as cracks. Nevertheless, the computational cost of a full 3D peridynamics analysis could be prohibitive. For this reason, researchers are working on coupling of local elasticity with peridynamics (i.e. [2,3]), in order to exploit the features of both theories. This work investigates crack propagation problems by combining local and non-local elasticity models. Specifically, the portion of the domain where the failure takes place is modelled via 3D peridynamics. On the other hand, the remaining part of the domain is modelled via refined 1D elements through the Carrera Unified Formulation (CUF) [4], which in recent years has proven to provide 3D-like results with a significant reduction of the computational cost. The coupling between the two domains is realized through the introduction of Lagrange multipliers, as presented in [5]. The present work is an extension of a previous one [6], where fracture in brittle material solid specimens was investigated through sequentially linear analysis. Particular attention is focussed on the crack propagation in multi-component structures (e.g., thin-walled reinforced structures) and multi-scale problems.

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Crack Propagation Analysis in Embankments during Earthquakes using Ordinary State-based Peridynamics

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Key Words: *Crack propagation analysis, Peridynamics, Embankment, Seismic response analysis*

An earthquake can induce the failure of soil embankments owing to the initiation and propagation of several cracks caused by extension stress and shear stress in these embankments. To improve the earthquake resistance of soil embankments, it is crucial to clarify the crack initiation and propagation processes. Peridynamics, a nonlocal formulation theory of continuum mechanics introduced by Silling [1], is a powerful method for such analyses. For applying seismic-response analysis to ordinary state-based peridynamics (OSB-PD), Shimbo et al. [2] formulated the seismic response analysis for crack propagation analysis using OSB-PD.

In the present study, a crack propagation analysis of a compacted clay embankment during an earthquake was performed. The physical parameters of the compacted clay were obtained via uniaxial compression tests with an initial crack. The compacted clay was assumed to be a linear isotropic elastic material with a bulk density (ρ_t) of 1761 kg/m^3, the Young's modulus (E) value of 8.5 MPa, a Mode II Fracture toughness (K_{IIC}) of 6.2 kPa.$\sqrt{}$m, and a critical stretch (S_c) of 0.0018. The input seismic wave was a sinusoidal wave with a frequency of 1 Hz and a maximum acceleration of 300 Gal, and the acceleration gradually increased according to the envelope curve. The analytical model used was an embankment-only model with a slope of 1:1.25, a height of 5 m, a crown width of 5 m, and a bottom width of 20 m. The bottom of the analytical model had a fixed boundary conditions in the horizontal and vertical directions. In the embankment-only model, the horizontal stress due to gravity was eliminated using the viscous boundary condition. In the present analysis, the seismic waves were input from the bottom of the analytical model after the stress distribution due to gravity was stabilized. To confirm that the stress distribution due to gravity was stable, the stress distribution was calculated using kernel interpolation.

The analysis of crack propagation during earthquakes shows typical failure patterns of embankments during the earthquakes, such as cracks in the slope and shear failure (i.e., a sliding surface) caused by the crack initiation and propagation.

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Dual Horizon Peridynamic Implementation in a Finite Element Framework - ANSYS

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Key Words: *Peridynamics, Dual-horizon, Non-uniform mesh, Finite elements, ANSYS*

This study presents a finite element framework to perform a dual horizon bond-based (BB), ordinary state-based (OSB) and non-ordinary state-based (NOSB) peridynamic (PD) analysis in ANSYS, a commercial software, with native MATRIX 27 elements. Especially in large-scale models, a non-uniform PD discretization leads to computational efficiency. However, non-uniform mesh with a varying horizon causes spurious wave reflections and ghost forces between the PD points due to the assumption of uniform horizon in the derivation of BB and state-based PD equilibrium equations [1, 2]. Ren et al. [3] introduced the concept of dual horizon PD to consider non-uniform discretization with a varying horizon. The PD equilibrium equations are satisfied only at points with a complete horizon. Otherwise, they are not satisfied at points with an incomplete horizon even for a homogeneous displacement field. This also results in residual forces leading to kinks and unphysical stress concentration near the boundaries. In order to remove this limitation, the domain can be split into three regions: interior, outer and boundary layer regions. The dual horizon BB, OSB and NOSB equilibrium equations can be considered at every point in the interior region with a complete horizon. The PD differential operator (PDDO) [4] or PD least square minimization (PD LSM) [5] form of the equilibrium equations and the traction components can be considered at a point with an incomplete horizon in the outer and the boundary layer regions. These equations permit the direct imposition of both displacement and traction boundary conditions in the boundary layer region. In each region, MATRIX27 elements native to ANSYS are employed to model PD interactions (bonds). The coefficients of the MATRIX27 element are expressed in terms of PD functions. Failure is introduced gradually as suggested through the EKILL option in ANSYS. The accuracy of the approach is demonstrated by considering a plate with or without a crack under tension subjected to various types of boundary conditions.

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Dual-horizon peridynamic element and its coupling with finite element

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Abstract

The peridynamic theory redefines the mechanical problems in terms of integral equations rather than partial differential equations, which makes it mathematically compatible with crack initiation and propagation. However, the surface effect and high computational consumption of peridynamics certainly limit its application. To make peridynamics widely available for numerical scientists and engineers, a potentially valuable method may be the integration of the PD and its coupling with FEM within the finite-element commercial software, such as Abaqus. To implement peridynamics in Abaqus, the dual-horizon peridynamic element is proposed and constructed in Abaqus/UEL. Correspondingly, the dual-horizon peridynamic element internal force vector and element stiffness matrix are derived and constructed. To implement the coupling model of PD and FEM in Abaqus, a unified variational weak form is proposed based on the convergence of peridynamics to the classical model in the limit of vanishing horizon. Since the integrals of the dual-horizon peridynamic element (DHPDE) and finite element in this dual-based coupling method are completely decoupled in the viewpoint of numerical implementation, which makes it easier to realize the adaptive coupling by switching integral element. Several numerical examples involving the static and dynamic crack propagation are investigated and the satisfactory results show the availability of the dual-horizon peridynamic element and its coupling with finite element. The implementation of DHPDE in Abaqus can fit into any existing computing platform and can be parallelized conveniently, which may make it easy for researchers and engineers to model engineering crack propagation in Abaqus.

Keywords: Dual-horizon peridynamic element; Abaqus/UEL; Unified variational weak form; Dual-based coupling method; Crack propagation.

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Improvements of Fracture Analysis on Shear Behaviours by Using Modified Ordinary State Based Peridynamics

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Key Words: *Fracture analysis, Peridynamics, Stress intensity factors, Shear deformation*

Ordinary state based peridynamic theory (OSPD), as one of the meshfree method, is widely applied in the fracture analysis nowadays. However, it has shown less accuracy in the simulations of shear behaviours in the fracture analysis. Therefore, a modified OSPD is introduced to improve the performance of the original theory. Different from original bond kinematics, deformations induced by bond rotation are taken into consideration. Meanwhile, the rigid body rotation (RBR) of the bond is also determined and removed from the total displacement with the help of peridynamic differential operator (PDDO) technique. The modified OSPD is tested by several typical benchmark problems. Stress intensity factors (SIFs) are evaluated by employing J-integral method. The numerical solutions of these cases are validated by the reference results provided in the literature and original OSPD. Good agreements of the solutions between the modified OSPD and reference methods can be derived. Meanwhile, the improvements in the mode-II fracture analysis have also proved accuracy and reliability of the proposed formulation in the simulation of shear fracture behaviours.

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Peridynamic Analysis of Porous Media with Micro-cracks

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Key Words: *Peridynamics, Porous media, Wave propagation, Micro-cracks*

Peridynamics [1] is a new continuum mechanics formulation. As opposed to partial differential equations of classical continuum mechanics, peridynamic equations are in integro-differential equation form and do not contain any spatial derivatives. Therefore, peridynamics is very suitable to analyse problems with discontinuities such as cracks. Moreover, peridynamics has a length scale parameter called horizon which allows representing non-local effects which cannot be captured by using classical continuum mechanics. There has been significant progress on peridynamics research especially during the recent years [2,3].

In this study, wave propagation in porous media subjected to impact loading is investigated by using ordinary state-based peridynamics. Moreover, the effect of micro-cracks on wave propagation is examined by changing the number of micro-cracks and their orientation. It is observed that depending on the micro-crack configuration, wave propagation can be significantly influenced due to the existence of micro-cracks.

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Peridynamic Simulations of Gas-pore Effects on Fatigue Lifetime

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Key Words: *Peridynamics, Fatigue lifetime, Gas pore, Additive Manufacturing*

Additive manufacturing (AM) becomes increasingly attractive in a wide range of industries, but it remains a tough task to understand its unique fatigue performance, which is mainly due to its intrinsic meso-defects such as gas pores and lack-of-fusions. Due to the complex impacts of interactive mechanisms between mechanics and materials, it is difficult to reveal the impacts by experiment or mechanical analysis. As an attempt, peridynamics (PD) is adopted in this paper to numerically study gas-pore effects on fatigue lifetimes of 2-dimensional smooth specimens.

While the computational costs of modeling meso-defect by reducing material point sizes for the smooth specimen is unacceptable, it is necessary to develop a multiscale modelling approach to map the meso-defect effects onto the upper scale. Thus, a strategy is developed by decomposing an origin PD bond into many sublevel bonds, and the status of PD bond can thus be more elaborately described as “how much works” rather than dualistic judgement of “broken or not”, whose capabilities are verified by comparisons with FEM results.

Combining such strategy with PD fatigue damage-cumulative model [1], numerical simulations are performed to reveal the gas-pore effects on fatigue lifetimes; to be specific, the gas-pore is approximated as circular meso-defect with three radius cases of 20,50,100μm, and its location varies from surface roughness to subsurface and to the interior. It is shown that the gas-pore location and size exert interactive impacts on fatigue lifetimes: a larger defect is of course more dangerous, but the threshold size below which the gas-pore effects on fatigue lifetimes is dependent on its specific location, and subsurface gas-pore is always the most dangerous place. To be more specific, data distribution degree of fatigue lifetimes is decided by gas-pore sizes, while data distribution shape of fatigue lifetimes is decided by gas-pore locations.

To conclude, this work provides a PD-based procedure as well as guidelines for AM processing optimization and understanding of meso-defect effects on fatigue lifetimes of AM materials. In the future work, more features such as defect shape, defect orientation and defect numbers can be considered, and the method can be extended to 3D cases.

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Simulation of Brittle/Quasi-brittle Fracture with the Smoothing Gradient Damage Model

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Key Words: *Brittle fracture, Quasi-brittle fracture, Gradient enhanced damage, FEM*

We present two fracture problems, anisotropic fracture and failure in rock-like materials. In the first part, we introduce a novel smeared gradient-enhanced damage model [1, 2] which takes into account directional-dependent damage evolution in two-dimensional polycrystalline materials. In details, the cleavage fracture in polycrystalline materials is considered. In terms of the recently developed smoothing gradient damage model [1, 2] for isotropic localized failure analysis, we introduce a new damage evolution equation to capture anisotropic fracture. Theoretically, directional fracture properties are integrated with the damage evolution equation through a second-order structural tensor [3]. The efficiency of proposed damage model is demonstrated through numerical experiments. The second part focuses on the analysis of mixed-mode fracture process of rock-like materials. For this problem, a novel equivalent strain formulation, developed in [4], is modified and integrated into the smoothing gradient damage model [1, 2]. We consider several popular rock fracture problems.

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Smoothed variable horizon Peridynamic modelling and its applications

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Key Words: *Peridynamics, Contact analysis, Dynamic fracture, Particle Method*

Peridynamics, one of particle method, has advantages for several fracture problems. On the other hand, many particles are required to ensure accuracy, compare with mesh based method, such as Finite Element Method. Furthermore, conventional peridynamics has the limitation that the horizon, range of influence function, should be same values. it leads the particles size is equal on entire model.

The variable horizon approach which supports the varying horizon, particle size, was proposed. However, the ghost force problem was detected. The ghost force is the discretization error, and it arises along the transition region of different horizon.

We have proposed smoothed variable horizon peridynamic model to reduce the ghost forces and it is adopted in this study.

In this study, the smoothed variable peridynamic concept extends to the contact model. The contact forces, short-range force in PD, was re-defined for varying horizon and the re-formulated the governing equation.

The Hertz problem is examined, and the numerical result converged to the theoretical. In addition, the computational cost was significantly reduced with variable horizon contact peridynamic model.

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A variational phase-field model for subcritical fracture

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Key Words: phase-field, subcritical fracture, stress corrosion

We present a variational phase-field framework for modeling subcritical crack growth in geological materials. Also known as static fatigue, this phenomenon is characterized by the occurrence of crack extension at stress levels substantially below those associated with the critical energy release rate, G_c. We assume that this is brought about mainly by stress corrosion, in which highly stressed material at crack tips is weakened due to chemical reactions in the presence of an environmental agent. Prior studies in the literature point to the existence of a nominal value of the energy release rate, G_0, below which subcritical crack growth does not occur. Above this threshold, the speed of crack extension can be related to the crack tip energy release rate via a power relation known as Charles' Law.

Following recent phase-field approaches for modeling fracture due to cyclic fatigue [1, 2], we incorporate the aforementioned behavior in the variational phase-field framework by scaling G_c with a function whose time rate of change depends on a quantity analogous to the energy release rate. Apart from the displacement and phase-field variables already present in the standard model for brittle fracture, no additional field unknowns are introduced in connection with static fatigue. Instead, an ordinary differential equation must be solved to determine the critical energy release rate evolution at each material point. The coupled system is solved numerically using a hybrid discretization that utilizes classical finite elements for the linear momentum conservation and cell-centered finite volumes for the energy balance governing phase-field evolution [3, 4].

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Modelling the evolution of large fracture networks

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Key Words: *Fracture modelling, Linear Elastic Fracture Mechanics, subcritical propagation*

Geomechanical simulation of fracture growth is a useful technique for predicting fracture density, distribution and geometry, with important applications in geomechanical engineering and subsurface flow modelling. However fracture networks developed across large geological structures (e.g. km-scale folds, faults or diapirs) may contain hundreds of thousands or even millions of individual fractures, so it is impractical to simulate each fracture directly.

We have therefore developed a method to apply basic geomechanical laws governing fracture propagation to cumulative density distribution functions which represent the fracture population as a whole. In this way, we can model the evolution of these functions through time without needing to create realisations of the individual fractures in the network. We use this method to model the evolution of layer-bound fracture networks across large geological structures. We assume that brittle layers such as sandstone or limestone beds contain an initial population of small microfractures. As a deformational strain is applied to the layer, a stress concentration will develop around the fracture tip which can be calculated by Linear Elastic Fracture Mechanics theory [1]. This will cause the fractures to grow, at a rate predicted by subcritical crack propagation theory [2]. Eventually the fractures will reach the top and bottom layer boundaries, after which they will grow laterally as elongated layer-bound fractures. By applying the fracture propagation rate equations to the cumulative density distribution function representing fracture density as a function of size, we can model the evolution of these functions through time [3, 4].

For a simple model with uniform and constant strain, we can derive analytical solutions, but for more complex models with laterally and temporally variable strain, we can discretise the model into cells and timesteps. As the fractures grow, they will interact, and we must include the effects of these interactions. We include two types of interaction in our model: intersection between perpendicular or oblique fractures, and stress shadow interactions between parallel fractures. The rate of fracture interaction is dependent on the fracture population, so this will also evolve through time. We calibrate the results of these models by comparing the resulting cumulative density distribution functions with those derived from dynamically generated DFNs.

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Utopia: an open-source software for large scale simulations of pressure induced phase-field fracture propagation

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Key Words: Phase-field methods, Fracture propagation, Solution methods, Software

Non-linear phase field models are increasingly used for the simulation of fracture propagation problems. The numerical simulation of fracture networks of realistic size requires the efficient parallel solution of large coupled non-linear systems. Although in principle efficient iterative multi-level methods for these types of problems are available, they are not widely used in practice due to the complexity of their parallel implementation.

Here, we present Utopia, which is an open-source C++ library for parallel non-linear multilevel solution strategies. Utopia provides the advantages of high-level programming interfaces while at the same time a framework to access low-level data-structures without breaking code encapsulation. Complex numerical procedures can be expressed with few lines of code, and evaluated by different implementations, libraries, or computing hardware. In this presentation, first we illustrate a globally convergent solution strategy designed to solve non-convex constrained minimization problems [1]. Second, we provide an overview of its implementation [2], and provide an overview of its parallel performance. Third, we provide examples of pressure-induced phase-field fracture propagation in large and complex fracture networks. Solving such problems is deemed challenging even for a few fractures, however, here we are considering networks of realistic size with up to 1000 fractures.

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Interaction Integral Method for Thermal Fracture of Magneto-Electro-Elastic Materials with Interface

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Key Words: *Magneto-electro-elastic (MEE) material, Crack, Interaction integral (I-integral), Thermal loading, Intensity factors*

Magneto-electro-elastic (MEE) materials, consisting of piezoelectric and piezomagnetic constituent phases, have received special attention from the research community owing to their specialized performance and coupled behavior under thermal, electric, magnetic and mechanical loads [1]. However, reliability issues due to fracture during service in the thermal environment still remain a major factor preventing their further development during service in the thermal environment. Complex interfaces between different constituents cause a great challenge to the fracture analysis of MEE materials [2]. In this work, considering the effect of the thermal loading, an interaction integral (I-integral) method [3] for an impermeable crack is developed to extract the crack-tip fracture parameters including stress intensity factors, electric displacement intensity factor and magnetic induction intensity factor of homogenous, nonhomogeneous and multi-interface MEE materials. Combined with the extended finite element method, the I-integral is adopted to solve several crack problems to show the accuracy and validity of the method. The influences of crack-face thermal boundary conditions, crack inclination angle and crack length are analyzed in homogeneous MEE material. Then, the I-integral values calculated by different integration domains agree well with each other for nonhomogeneous and discontinuous material properties. Besides, good results show the effectiveness and the domain-independence of the present method in the fracture analysis of nonhomogeneous and discontinuous MEE materials. In view of the wide applications of MEE materials in various thermal environments, the present analysis could serve as a reference for the design of various smart structures of MEE media.

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Mixed finite-element formulations for flexoelectricity in piezoelectric solids with analysis of fracture behaviour

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Key Words: flexoelectricity, fracture mechanics, strain gradients, higher order theory, mixed FEM

Piezoelectricity is an important phenomenon observed only in certain classes of dielectrics. Conventional electromechanical coupling is restricted to material with a non-centrosymmetric unit cell structure. As an alternative, the flexoelectric effect is observed in all dielectrics and is prominent at micro- and nanoscales. Flexoelectricity is an electromechanical coupling between electrical (mechanical) quantities and strain (polarization) gradient. Flexoelectricity is a suitable substitute for piezoelectricity for electromechanical coupling and can be used for applications in nanosensors, actuators, high precision devices, etc.

Traditional continuum models lack material length scales which were introduced by Cosserat using strain gradients and significantly extended by Mindlin [1]. Strain Gradient Elasticity (SGE) theory results in fourth-order partial differential equations demanding C^1 continuous elements for traditional FEM to be used. To avoid such difficulties, mixed-FEM is used as formulated by Amanatidou [2] for SGE problems and later extended to flexoelectricity in dielectric solids by Mao [3] presenting I9-87 element (87 DOF).

In our work, a piezoelectric contribution is considered in addition to pure linear dielectric material in the formulation of flexoelectricity. This allows to clearly separate the influence of the piezoelectric and flexoelectric electromechanical coupling. As a particular case, when neglecting piezoelectric contribution, our results simplify to that of [3]. Additionally, in the vicinity of sharp tips (presence of cracks or defects), naturally occurring inhomogeneous strain distribution induces strong polarization even under the influence of a weak electric field. Our solution was implied for the crack problems, studying the mutual influence of the piezo- and flexoelectric contributions on the fracture parameters within the framework of the linear elastic fracture mechanics.

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Phase Field Modelling of Coupling Evolution of Fracture, Dielectric Breakdown and Polarization in Ferroelectric Materials

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Key Words: *Ferroelectrics, Fracture, Dielectric breakdown, Domain switching, Phase field model, Generalized configurational force*

Ferroelectric materials have attracted increasing attention due to their distinguished electromechanical performance. In the presence of mechanical and electrical loadings, the failure behaviours of fracture and dielectric breakdown may occur simultaneously in ferroelectric materials. Understanding the coupling evolution of fracture, dielectric breakdown and polarization is crucial for the application of ferroelectric materials under complex electromechanical environments. In the present study, a phase field model is developed to investigate the coupling evolution behaviour of polarization, fracture and dielectric breakdown in ferroelectric materials subjected to the mechanical and electrical loadings. Different degradation functions are proposed to model different interface boundary conditions for fracture and dielectric breakdown. Generalized configurational forces for fracture and breakdown are derived from the phase field model to analysis the driving forces for the coupling evolution. Under a set of interface boundary conditions, interactions between fracture and dielectric breakdown are investigated systematically. The phase field simulations show that dielectric breakdown can be induced by the concentrated electric field at impermeable crack tips. At the same time, the dielectric breakdown can influence the stress distribution around the crack tip as well as the driving force for crack propagation. The attraction of fracture to breakdown path and the deviation of breakdown to fracture path are observed simultaneously during the coupling evolution of fracture and breakdown. The results in the present work provide an insight into fracture and breakdown coupling failure mechanism in ferroelectric materials. The developed model framework can be employed to investigate more complex coupling failure behaviours of ferroelectric and dielectric materials.

Configurational Mechanics for Modelling Fracture Propagation in Heterogeneous and Anisotropic Materials

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Key Words: *Fracture, Configurational Mechanics, Heterogeneous Materials*

A mathematical formulation and numerical modelling framework for brittle crack propagation in heterogeneous elastic solids is presented. The formulation is developed in the framework of configurational mechanics and solved numerically using the finite element method.

The proposed model is based on the assumption of maximal dissipation of energy and uses the Griffith criterion. We show that this is sufficient to predict crack propagation in brittle heterogeneous materials, with spatially varying Young's modulus and fracture energy, and for anisotropic materials. The configurational forces and fracture energy release rate are both expressed exclusively in terms of nodal quantities, avoiding the need for post-processing, and enabling a fully implicit formulation for modelling the evolving crack front and creation of new crack surfaces.

For heterogeneous materials, it is shown that it is necessary to have a spatially smooth density field, with higher regularity than if the field is approximated directly on the FE mesh. Therefore, density data are approximated as a smooth field using a Moving Weighted Least-Squares method. For functionally graded materials, the density fields were generated analytically. Fracture in bone is also investigated, with density fields determined from clinically available CT scan data.

The proposed formulation is verified and validated by comparing numerical results with both analytical solutions and experimental results. Both the predicted fracture path and load–displacement response show very good agreement with experiments.

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Modelling Rock Fracture using the Stochastic Bonded Discrete Element Method

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Key Words: Bonded Discrete Element Method - Rock Fracture - Heterogeneous

Numerical modelling of the fracture of heterogeneous brittle materials is of interest for several industries, such as rock excavation and comminution applications. A numerical model of brittle materials needs to be able to capture the unpredictable results, e.g. with regards to measured strength and fracture pattern, as observed experimentally. In a previous work [1], the Bonded Discrete Element Method [2] was combined with statistical methods in order to generate heterogeneous rock bodies. Grains of random sizes and shapes, consisting of multiple bonded discrete elements, were generated in the body and the micromechanical parameters of these grains were governed by the Weibull distribution [3]. In this work, this modelling approach was used to evaluate the fracture behaviour of experiments commonly found within the field of rock mechanics - the unconfined and confined axial compression test, Brazilian disc test and the three point bend test. For each test, a large set of numerical samples were generated and simulated. The fracture behaviour, e.g. initiation, propagation and coalescence of cracks, were investigated for different levels of heterogeneity and grain cement strengths. The results show that a variety of different fracture modes can be obtained with this modelling approach. Further, the results suggests that the statistical methods employed in this work improves the versatility of the Bonded Discrete Element Method for rock modelling.

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Surrogate-based stochastic optimization for enhancing interfacial fracture resistance of heterogeneous structures

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Key Words: Interfacial Fracture, Surrogate-based Optimization

Recent developments in the field of computational modelling of fracture have opened up possibilities to design structures against failure. A special case, called interfacial fracture, can occur in loaded heterogeneous structures where two or more materials are bonded together at comparatively weak interfaces. Due to the presence of unstable crack growth along interfaces, the structural problem suffers from high nonlinearities and instabilities, leading to noisy and discontinuous responses. In such a case, local-gradient-based optimization approaches are not feasible due to lack of analytical sensitivities and also due to the presence of spurious local optima (minima). In this work, we use a stochastic optimization approach to maximize the expected value of the mechanical work done by external loads under uncertainties in the design parameters, distributed normally. To overcome the intractability of Monte-Carlo methods for the estimation of the expected value of the expensive-to-evaluate response function, an approximate global Voronoi-piecewise surrogate [1] is constructed using a few initial randomly generated samples. The surrogate function is refined successively in each optimization iteration by adding samples in a small region in the design space close to the current iterate. A local minimum of the expected value of the surrogate then results in the next design point. For the stochastic optimization of cheap-to-evaluate surrogate function, a Newton-type algorithm is used. Promising results show that by taking a large sampling region in the beginning of the optimization run and gradually decreasing it helps to overcome spurious local minima and leads to a robust final design. We show the effectiveness of the proposed framework with the help of optimization examples with up to 12 design degrees of freedom, where the shape parameters of the heterogeneities are optimized for interfacial fracture resistance. Finally, we show that the performance of the optimization algorithm can be significantly improved by reducing the dimensionality of the stochastic variables while keeping the dimension of the design parameters the same.

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Unified definition of stress intensity factors of a sharp three-dimensional jointed corner among dissimilar anisotropic materials

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Key Words: *Three-dimensional corner, Jointed anisotropic dissimilar materials, Eignevalue, Eigenfunction, Scalar parameters, Stress intensity factor*

In the manufacture of electronic devices and micro-electro-mechanical systems (MEMS), a wide variety of materials are jointed. For light-weight automobiles, CFRP materials are jointed with metallic materials. In these products, jointed interfacial corners are singular stress points from which fractures sometimes originate.

Evaluating the severity of singular stress fields is important for protecting these corners from fracture. In our previous studies, we proposed a definition of the stress intensity factors (SIFs) of two-dimensional (2D) jointed interfacial corners [1, 2]. We can use this SIFs formula to evaluate the singular stress field around a jointed interfacial corner with a smooth edge front in a three-dimensional (3D) object.

However, fractures sometimes occur from sharp 3D jointed corners. In our previous paper, we proposed a numerical method for calculating the scalar parameters (SPs) that describe the singular stress fields around sharp 3D corners [3, 4]. The SPs are the coefficients in William's Eigenvalue expansion form that express the singular stress field around a sharp notch or crack. In this study, we propose a unified definition of SIFs at sharp 3D jointed corners between anisotropic dissimilar materials. These SPs can describe the singular stress field, but they are not adequate as the fracture mechanics parameters which evaluate the fracture from such a corner.

In this study, we propose a new definition of the SIFs of a sharp 3D corner. The definition is compatible with the SIFs of 2D corners, of interfacial cracks and of cracks in uniform material. Furthermore, the proposed SIFs can describe the singular stress along any directions around a sharp 3D jointed corner.

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3D Meso-Scale Numerical Experiment of Reinforced Concrete Reflecting the Geometry of Deformed Bars and Coarse Aggregates

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Key Words: *3D Fracture Simulation, Meso-Scale, Numerical Experiment, Coarse Aggregate, Concrete, Damage Model*

Numerical experiments are carried out for reinforced concrete in 3D meso-scale. The reinforced concrete model reflects the geometry of deformed bars and coarse aggregates in detail. The damage model based on fracture mechanics of concrete is applied to crack propagation analysis of concrete and the von-Mises plasticity model is applied to the elastic-plastic analysis of steel [1]. The numerical experiments are compared to actual experiments performed in a laboratory. These results show good agreements, implying that the numerical experiments proposed in this study are physically reasonable.

The numerical experiment consists of a non-linear finite element analysis and 3D meso-scale reinforced concrete model. The finite element analysis with non-linear material models is first formulated. The modified von-Mises damage model based on fracture mechanics of concrete [2] and the standard von-Mises plasticity model are applied to the constitutive law of concrete and steel, respectively. The modelling of 3D meso-scale reinforced concrete is second explained. In particular, the detailed geometry of deformed bars and coarse aggregates is reflected in 3D. The 3D complicated spatial arrangement of coarse aggregates is also reproduced in detail.

We finally show numerical experiments of reinforced concrete beams with or without shear reinforcements to verify the availability of the proposed model. The numerical results are compared to experimental results performed in a laboratory. The comparison demonstrates that the numerical responses are in good agreement with those obtained experimentally. In addition, these results confirm that the failure modes simulated in the numerical experiments provide good fits to the experimental data.

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A 3D Model Combining Cohesive Zone Approach and Friction to Model the Steel-Concrete Interface

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Key Words: *3D cohesive zone model, Friction, Steel-concrete interface, Pull-out test*

It is essential to model the behavior of the interfaces between steel reinforcement and concrete in order to understand the stress transfer between these two components in reinforced concrete structures. The interface models commonly used include several parameters whose identification is based on pull-out tests, for which sensitivity to a number of parameters is not fully explained [1]. In this contribution, the steel-concrete interface is studied at the mesoscopic scale through the simulation of pull-out tests. The three dimensional numerical reinforced concrete samples are generated by applying the procedure described in [2], in which each sample is made up of concrete surrounding a ribbed or smooth bar embedded in the center of a cubic sample. The detailed geometry of the ribs of the steel bar is modelled with different possible shapes. Then, the finite element code Cast3M [3] is used to perform the pull-out numerical simulations on the generated samples, using Mazar's damage approach [4] with regularization to describe cracking in concrete. The steel-concrete interface is modelled by combining a modified cohesive zone model (CZM) based on Tvergaard's approach and a frictional model accounting for the frictional behavior in the damaged part of the interface. This is done by modifying the 2D approach described in [5] and generalized to 3D in [6], by replacing the Crisfield's damage model by the more adapted Tvergaard's model and modifying the corresponding stresses to account for its exponential behavior. The interface is divided into an undamaged part where the CZM model applies and a damaged part where the frictional model dominates. The total stress is then the addition of the two corresponding stresses, and is equivalent to the CZM stress when the interface is initially undamaged, and fully equivalent to frictional model's stress when the joint element is finally fully damaged. The overall response is studied in terms of the damage near the steel bar, the applied force versus displacement curves, and free end displacements. The results of mean bond stress versus the free end displacement are compared to available experimental data.

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A variational formulation for thermally-induced cracking in concrete

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Key Words: *Variational formulation, Thermally induced crack, Concrete, Thermo-mechanical coupling, Continuum damage mechanics*

Fracture phenomena of concrete have been investigated in various aspects, and many models have been developed to predict crack initiation and propagation under a variety of mechanical and/or environmental conditions. In particular, thermo-mechanical coupled problems have seen some standard formulations for thermally induced cracking in concrete, but as far as we know, not yet been formulated as a variational problem based on fracture mechanics. To this end, in this study, a novel variational formulation for thermally induced cracking in concrete is originally presented. Specifically, we formulate the variational problem for a continuum damage model based on fracture mechanics that is coupled with heat conduction and realize thermally induced cracking phenomena in concrete by implementing it in our finite element (FE) code.

As the first step, we define a Helmholtz energy function and a damage "yield" function based on the isotropic damage model proposed by Kurumatani et al. [1] that is consistent with the conventional cohesive zone model. Next, in line with Canadija & Mösler [2], a functional of total energy rate and its optimization problem is formulated to obtain the equilibrium state of concrete. Finally, optimality conditions are established to derive the weak form and the load/unload conditions for damage evolution and heat conduction. After the suitable discretization for time and space within the FE framework, the resulting equations are properly implemented. The capability and merit of proposed formulation against the convetional formulation by presenting representative numerical examples to predict the thermal-induced cracking in concrete structures.

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Phase-field Modeling for Damage in Reinforced High Performance Concrete at Low Cycle Fatigue: Numerical Calibration and Experimental Validation

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Key Words: high performance concrete (HPC), steel-fiber reinforcement, phenomenological material model, elasto-plastic phase-field model, three-point bending beam test, degradation of residual stiffness

High performance concretes (HPCs) have attracted a great interest in the construction industry worldwide because of its wide variety of applications. The dense microstructure of HPCs and additional reinforcement of steel fibers gives high strength and superior durability, see [2]. These additional fibers restrain the further growth of crack by transmitting the stresses from concrete matrix to fibers during fracture which affects the deterioration characteristics of concrete in cyclic flexural tests, see [3]. On this account, within DFG priority program 2020 (SPP 2020), strong research is focused on the experimental and numerical analysis of failure of HPC under fatigue. In this contribution, a phenomenological material model is developed combining the superposed models of transversal isotropic elasto-plasticity, see [1] and a continuum phase-field model based on the variational formulation of fracture in elasto-plastic material, cf. [4, 5, 6]. Two different data driven degradation functions for the modeling of unique behavior of HPC in tension and compression are calibrated by simulating the typical uniaxial cyclic tests. The numerical model is calibrated and validated by comparing the numerical results of three-point bending beam test at low cycle for pure and reinforced HPCs to experimental data, see [7].

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Study on Damage Characteristics of Ceramsite Concrete Based on Multi-phase Mesoscopic Model

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Key Words: *Ceramsite Concrete, Multiphase Mesoscopic Model, Lattice Model, Interfacial Transition Zone, Damage analysis*

As a novel building material, lightweight ceramsite aggregate concrete has been widely used in the construction of high-rise buildings, long-span bridges, and marine structures in harsh environments as the obvious advantages in its lightweight, good thermal properties, fire resistance, and seismic resistance as well as environmental friendliness. In this paper, a lattice model for mesoscale modelling of heterogeneous materials was proposed, and the mesoscopic damage mechanism of ceramsite concrete was studied. The mesoscopic multiphase lattice model was established by mapping the random aggregates model onto the random disordered grid, and the correctness of the model was verified by comparing it with the experiment. Based on the Mazars damage constitutive relation, the damage failure mechanism of ceramsite concrete was studied. The damage of ceramsite concrete first occurred in ceramsite as the ceramsite aggregate was the weakest composition in ceramsite concrete composite, which is different from the damage first appearing in the interface transition zone of ordinary concrete. Then, the damage evolution of ceramsite concrete could be expressed as: with the application of load, the damage appeared discretely in a number of ceramsite aggregates and involved into micro cracks in some aggregates. As the applied load continued to increase, the damage gradually developed to the ITZ and cement mortar area. When the applied load reached its peak, the damages began to fuse and initially developed into a macrocrack. With further loading, the macrocrack developed rapidly as the damage evolution intensified around the macrocrack while relieved in the other region.
The proposed multi-phase mesoscopic lattice damage model can accurately calculate the whole deformation and failure process of concrete at a low cost, especially, the proposed model can effectively simulate the strain-softening and damage localization of concrete materials.

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3D dynamic fracture analysis using high-order elements of SBFEM

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Abstract

A time-domain method for modeling three-dimensional dynamic fracture using high-order elements [1] of the scaled boundary finite element method (SBFEM) is presented. The scaled boundary finite element method can simplify the modeling of cracks and extract the dynamic stress intensity factors directly from sigular stress field around the crack tip, which shows great potential for fracture analysis [2,3]. The spectral element approach [4] and hierarchical polynomial shape functions [5] are applied to generate the high-order shape functions of elements. The mass and stiffness matrix of high-oder elements are derived based on the high-order shape functions [6,7]. The three-dimensional equation of motion are established and solved by using the Newmark method. Linear ealstodynamic fracture mechanics is used to define the dynamic stress intensity factors (DSIFs) [8], which are directly extracted from the dynamic response at each time step. A benchmark problem is investigated to validate the accuracy of high-order elements. Numerical results demonstrate that both the p-refinement and h-refinement can improve the computational accuracy of the DSIFs. It is proven that higher rate of convergence is obtained using p-refinement instead of h-refinement.

Key Words: Dynamic frature mechanics, Scaled boundary finite element method, Three-dimensional dynamic stress intensity factors, High-order elements, p-refinement, h-refinement

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A Massively Parallel Solver for Explicit Damage Analysis Exploiting Octree Mesh Patterns

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Key Words: *Octree mesh, Explicit damage analysis, Parallel computing, Scaled boundary finite element method.*

This work develops a massively parallel solver for performing explicit damage analysis of structures in three dimensions. To eliminate the mesh sensitivity due to strain localisation, an integral-type non-local model is implemented. The problem domain is discretised using balanced octree meshes. The repeating cell patterns are exploited for the pre-computation of element matrices leading to lesser memory requirements. The scaled boundary finite element method (SBFEM) is employed, which directly handles octree cells as polyhedral elements and eliminates the hanging nodes issue. To efficiently perform the matrix operations associated with solving equilibrium equations, an element-by-element (EBE) approach is utilised. Here, the reduced number of unique octree patterns are exploited to perform group-wise matrix computations, which avoids a global matrix assembly, allows better cache utilisation, and aids associated memory-bandwidth limited computations, resulting in significant performance gains. The parallelisation is carried out using the mesh-partitioning strategy and implemented using the message-passing algorithm. The developed computational framework can efficiently simulate large scale damage problems with more than a hundred million unknowns and allows for massive scaling with several thousand cores in a distributed computing environment.

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A NURBS enhanced polygonal element formulation for the nonlinear analysis of solids in boundary representation

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Key Words: Polygonal element formulation, Scaled boundary finite element method, Displacement elemnent formulation, Nonlinear solid mechanics

The contribution is concerned with a numerical element formulation for the nonlinear analysis of solid in boundary representation. Its results in a polygonal element with an arbitrary number of sides. Straight edges are possible as well as curved edges, which are described by e.g. Non-Uniform Rational B-Splines (NURBS).

The presented element formulation is based on the scaling concept, which is adopted from the so-called scaled boundary finite element method (SBFEM), see [2]. The SBFEM is a semi-analytical formulation to analyze problems in linear elasticity. Within this method the basic idea is to scale the domain's boundary with respect to a scaling center in order to describe the interior domain. In contrast to SBFEM, the proposed method uses a numerical approximation for the displacement response in scaling direction. This enables the analysis of geometrically and physicallly nonlinear problems in solid mechanics, see [1]. The interpolation at the boundary in circumferential direction is independent of interpolation in scaling direction. This allows the use of different basis functions for each direction, e.g. NURBS basis functions in circumferential and Lagrange basis functions in radial direction.

The advantage of the presented element formulation is the flexibility in mesh generation. For example, using Quadtree algorithms, a fast and reliable mesh generation can be achieved. Furthermore, in connection with trimming algorithms, the element formulation allows a precise representation of the geometry even with coarse meshes. Some benchmark tests are presented to evaluate the accuracy of the proposed numerical method against analytical solutions, and a comparison to standard element formulations is given as well.

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A Scaled Boundary Finite Element Framework for Mesh Burden Alleviation and High-Performance Computing

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Key Words: *Scale boundary finite element method, Polyhedron element, Octree, High-performance computing, Explicit dynamics, Preconditioned conjugate gradient solver*

In the scaled boundary finite element method [1], an element is constructed semi-analytically. The boundary is discretized and the solution inside the element is obtained analytically. Within this framework, the element can take *any* shape and it only needs to satisfy a scaling requirement (i.e. there exist a point from which the whole boundary is directly visible). The scaled boundary finite element method provides a high degree of flexibility in terms of element shape and order. It has been shown to be highly complementary with the octree meshing algorithm. The combination is capable of significantly alleviating the mesh burden for not only the conventional CAD models but also digital images [2] and STL models [3]. The boundaries can be defined either explicitly by the elements or implicitly embedded within the elements [4]. It is found that the number of unique element patterns in an octree mesh is limited to a very small number and the operation of a matrix-vector product can be performed efficiently according to the patterns of the polyhedron elements on a high-performance computing (HPC) facility. The potential of this approach is demonstrated by an explicit time integration scheme [5]. Based on the same technique, a preconditioned conjugate gradient solver is developed for HPC. The implicit time integration scheme can be performed like an explicit scheme, retaining the advantages of both schemes. The extension to consider material nonlinearity is also addressed. Numerical examples are presented to demonstrate the concept and potential of the proposed framework.

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A temporally piecewise adaptive extended multiscale scaled boundary finite element method for viscoelastic problems

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Key Words: *multi-scale; viscoelastic promble; temporally piecewise adaptive algorithm; numerical base function.*

This paper provides a new numerical method for solving multi-scale heterogeneous viscoelastic problems which is presented by combining the extended multi-scale scaled boundary finite element method and the temporally piecewise adaptive algorithm. In the time domain, temporally piecewise adaptive algorithm is adopted and the recursive equations for solving multi-scale viscoelastic problems are derived. When the time step changes, the computation accuracy in time domain can be guaranteed by adaptive calculation. In the space domain, the extended multi-scale scaled boundary finite element method based on numerical base function is used to solve the recursive equation and decrease the solution scale. The stress singularity can be easily and effectively dealt with. Combined with quadtree technique, the meshing of scaled boundary finite element based on image recognition is realized. The proposed approach provides a flexibility to increase macro scale nodes without increasing new nodes inside the coarse element and changing the shape of the fine grids according to the position of the increase macro nodes. The solution accuracy can be improved by such an increase. Numerical examples show that the proposed method has stable accuracy and can effectively improve the computational efficiency.

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Crack-like Defect Inversion Model Based on SBFEM and Deep Learning

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Key Words: *non-destructive testing, scaled boundary finite element methods, deep learning, inverse problems, defect identification, crack*

The identification of structural internal defects is an important research content of structural health monitoring. At present, the structural safety inspection based on non-destructive testing mainly focuses on qualitative analysis, so it is difficult to identify the scale of defects quantitatively. In this paper, an inversion model is proposed by combing the scaled boundary finite element methods (SBFEM) [1-2] and deep learning [3-4]. The identification of crack-like defects can be performed in structures based on the feedback signal of Lamb wave propagation. By randomly generating defect information, i.e. position and size, the SBFEM can be used to simulate the signal propagation process of Lamb wave in structures with defects. The SBFEM only needs to discretize the structure boundary, which can minimize the re-meshing process and greatly improve the computational efficiency. When Lamb wave propagates in a cracked structure, the feedback signal of the observation point can reflect crack information. Based on this characteristic, enough training data reflecting the characteristics of the problem can be provided for the deep learning model. The proposed defect inversion model avoids the iterative process of minimizing the objective function of the traditional inverse problems [5], and greatly reduces the computational cost on the premise of ensuring accuracy. Numerical examples of plates with single and multiple cracks are analyzed. The results show that the defect identification model can accurately quantify the defects in the structure. It also has a good identification effect for shallow cracks. The model also shows robustness to the noisy signal model.

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Differentiation of a scaled boundary finite element model in the context of material parameter determination

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Key Words: Differentiation, Guided Waves, Scaled Boundary Finite Element Method, Optimization

The task of frequency-dependent material parameter determination in the ultrasonic regime is established as an inverse problem relying on measurement and simulation data. The latter is provided by a forward model, which must be repeatedly evaluated; thus, a high-performance model is required. Especially in the case of cylindrical samples, the (axisymmetric) scaled boundary finite element method (SBFEM) provides a framework to derive such an efficient model. The number of degrees of freedom is reduced to a minimum by discretizing only along the radial direction while permitting the computation of bounded domains of arbitrary length [1].

The inverse problem is interpreted as an optimization problem w.r.t. the differences between measured and simulated mechanical displacement responses. While global optimization allows finding a global minimum, it requires an excessive number of model evaluations, and thus is not considered in this work. In contrast, given adequate initial parameters, local optimization, specifically gradient descent, is favored because it promises fast convergence. However, an accurate computation of gradients requires differentiation of the forward model with respect to the parameters that are to be determined.

In this contribution, we present the explicit differentiation of the SBFEM model via iterative application of the chain rule. We discuss the challenges faced in the differentiation of the Hamiltonian eigenvalue problem, which is an essential part of the SBFEM formalism [2]. Our method leads to a robust and efficient computation of gradient information far superior to the application of finite difference quotients.

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Dynamic crack face contact based on the scaled boundary finite element method

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Key Words: *Scaled Boundary Finite Element Method, Dynamic Crack Face Contact*

The static and dynamic contact problems of general structures have been widely studied. However, regarding crack problems, due to the singularity of the stress at the crack tip and the complexity of the dynamic contact on the crack faces, only a few studies have considered the dynamic contact on the crack face.

The scaled boundary finite element method is used to solve dynamic crack face contact problems. Ooi et al. [1] constructed bubble functions based on the displacement field that would be caused by polynomial body loads. The method is applied to the problem of crack side-face loads. The scaled boundary finite element (SBFE) shape function considering the side-face loads is used to derive the dynamic contact equation and the characteristic matrix related to the dynamic calculations [2].

The standard Newmark time integration algorithm is very successful in analyzing the conventional dynamic responses of structures, but its application in the Lagrange multiplier method meets some difficulties in dealing with dynamic contact problems effectively [3]. Especially when time step Δt is very small, the classical Lagrange multiplier method will give out the oscillatory field of contact forces. A modification of the classical Lagrange multiplier method is presented using a special time integration.Due to the introduced high-frequency dissipation in this time integration algorithm, this method can lead to the effective analysis of real response of elastic bodies with dynamic crack face contact constraints. The results show that this method has higher precision than the traditional Newmark time integration algorithm.

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Finite Element Method with Optimal Functions (FEM-OF)

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Key Words: *Domain Decomposition, Discontinuous piecewise-defined functions*

The current connotation of domain decomposition is to divide a global problem into several independent local problems to apply parallel computing. But in a broad sense, domain decomposition refers to a systematic way of introducing a partition, so that functions can be defined in each of its elements independently, thus generating a linear space of piecewise discontinuous functions. When working in these spaces, the problem to be solved is called the Boundary Value Problem with Prescribed Jumps (BVPJ) [2].

As a background, Dr. Herrera and his collaborators, based on an Algebraic Theory applied to Boundary Methods, which generalizes Green's formula to linear spaces of piecewise discontinuous functions, have developed two discretization methods [1]. The first one, called the Direct Method (or Poincaré-Steklov Method), arises from the weak formulation in terms of the data of the problem; while the second one, called Indirect Method (or Trefftz-Herrera Method), arises from the weak formulation in terms of the complementary data of the problem. The difference between them is the following. In the first one, local solutions of the homogeneous differential equation are developed in each element of the partition to construct specialized base functions called optimal base functions; while in the second one, local solutions of the homogeneous adjoin differential equation are developed in each element of the partition to construct specialized weight functions called optimal weight functions. In practice, the optimal functions are approximated with numerical methods; for example, Collocation Methods.

In this work, a novel method is presented that articulates the aforementioned methods by means of a dual decomposition of operators, which simultaneously uses the optimal base functions and the optimal weight functions. The dual decomposition of operators is determined by what is called the sought information from the solution in the interior boundary, which could be either the average of the function, or the average of its normal derivatives. This method has been called the Finite Element Method with Optimal Functions (FEM-OF), since the optimal functions are approximated with the conventional Finite Element Method. In this way a general basis for a theory of finite element methods in spaces of piecewise discontinuous functions is established. In the general literature, methods that use different spaces for base functions and weight functions are called Petrov-Galerkin Methods.

The FEM-OF method has a great generality because it can be applied either to linear differential equations or to systems of them. In this work, applications to the general second-order equation and linear elasticity equations are presented. FEM-OF has significant advantages over conventional FEM. Two of the main advantages are that FEM-OF reduces the number of degrees of freedom and that it exhibits superconvergence when applied to non-self-adjoint differential operators. Other advantages are that FEM-OF generates better structured matrices, it has a great flexibility to select the approximate polynomial spaces and, as already mentioned, that it can be applied without additional difficulties to BVPJ. In any case, FEM-OF has higher precision.

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High-frequency scattering analyses at dramatically low computational cost using phase-reduced isogeometric on surface radiation conditions

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Key Words: acoustic scattering, on-surface radiation condition, isogeometric analysis, Non-convex scatterers, phase reduction

We develop Isogeometric on surface radiation condition (IGA-OSRC) method to solve acoustic scattering problem. First, we demonstrate the possibility of reducing the spatial dimension by one and alleviation of mesh burden using the proposed IGA-OSRC. Geometrical features were evaluated accurately even at very course discretization levels. The Pade-type OSRC was optimized to increase the accuracy of the proposed method especially at high frequency analyses. To avoid pollution error and enable dramatically fast analyses at high frequencies, we separate the oscillatory part of the solution and solve for slowly varying amplitude leading to development of phase-reduced IGA-OSRC (PR-IG-OSRC). We demonstrate the performance of the PR-IGA-OSRC method for two- and three- dimensional acoustic scattering problems and propose a coupling method to increase its accuracy for analyses of nonconvex scatterers. Hence, the proposed method reduces the meshing burden, increases the accuracy, and dramatically reduces the computational cost for the analyses of arbitrary shaped scatterers.

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Modelling Creep in Short-Fibre Reinforced Composites Based on the Scaled Boundary Finite Element Method

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Key Words: Creep, Scaled Boundary Finite Element Method, Rate-Dependent Inelasticity, Image-Based Analysis

Nowadays, short-fibre reinforced composites (SFRCs) have been established for a variety of applications. However, many matrix materials, such as concrete or polymers, exhibit rate-dependent inelastic behaviour ("creep"). Since the microscopic behaviour of composites determines their macroscopic response, it is crucial to consider the complex microstructure in detail. It is possible to use the finite element method (FEM) to analyse SFRCs. Nevertheless, creating a conforming mesh for the fibres and matrix with the FEM is usually time-consuming and might also require additional constraints. In contrast, the scaled boundary finite element method (SBFEM) is ideally suited for a fast image-based discretization of microstructures because because the spatial discretization can be directly constructed by utilising the efficient quadtree-decomposition technique. Note that the SBFEM has already been successfully applied to model the elastic behaviour of SFRCs in Ref. [1]. Furthermore, it has been extended to inelastic behaviour for plasticity in Ref. [2] and rate-dependent inelasticity in Ref. [3].

The current contribution combines both approaches: First, a new non-linear constitutive model for basic creep of concrete is introduced. The model is implemented into an SBFEM framework by performing the stress update algorithm only at the scaling centre of the polytopal elements to increase the numerical efficiency. Second, creep of short-fibre reinforced concrete is modelled, whereas the new constitutive model is used for the concrete matrix. In contrast, a linear isotropic elasticity model is chosen for the fibres. The contribution at hand makes use of image-based analysis to generate meshes based on microstructural images. By means of various examples, the accuracy and efficiency of the proposed approach are numerically demonstrated.

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Nonlocal Macro-micro Damage Model For Cracking Simulation Based On SBFEM

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Key Words: *scaled boundary finite element method, a quadtree mesh, nonlocal macro-micro damage model, an energetic degradation function, cracking simulation, damage*

Combined with the unified phase field theory and the concept of peridynamics, a novel nonlocal macro-micro-scale consistent damage model is proposed to simulate fracture process without prescribed initial crack and potential crack path. The model introduces the relative deformation of material point pair to describe the microscopic damage inside the structure, and then the macro-scale topologic damage is evaluated as the weighted averaging of micro-scale damage over bonds in the influence domain [1]. Since the size of the element in the damage area is small enough, it is assumed that the damage is evenly distributed in an element [2]. An energetic degradation function, which connects the energy-based damage and the macro-scale topologic damage, is introduced to consider the stiffness reduction caused by the damage, so that the topological damage can be conveniently embedded into the calculation of the global stiffness. Finally, the nonlocal macro-micro damage model is coupled into the framework of scaled boundary finite element with the scaling center as the material point. A quadtree mesh was used to refine the damage process area, and the advantage of scaled boundary finite element mesh allowing hanging nodes were fully utilized to obtain multilevel mesh effectively [3]. The model achieves efficient calculation from material point pair deformation to topological damage and reduces the computational workload and time effectively. Several numerical examples show that the proposed model can capture not only the crack pattern but also the load-deformation curves quantitatively, and model also has better computational accuracy and efficiency than the existing model. Results also indicate when the size of the element in the damage area is less than 1/5 of the radius of the influence domain, there is no mesh sensitivity in the calculated results.

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Pointwise conservative SBFEM approximations based on mixed finite elements

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Key Words: SBFEM, Mixed FEM, $H(div)$ function spaces, Darcy Flow

In many engineering simulations, the divergence-free conditions of the approximation are perceived as an essential characteristic of the numerical method. Such conditions are common in incompressible fluid models and hard to impose using classical H^1 approximations. $H(div)$ approximations when combined with De Rham compatible L^2 approximations lead to pointwise divergence-free approximations.

The SBFEM method is known to yield convergent approximation spaces even when the geometry of the domain induces singularities, such as crack tips and re-entrant corners. The difficulty of approximating partial differential equations for such geometries is because the usual shape functions are based on polynomial interpolation functions and these lead to suboptimal converge rates. In this context, the Scaled Boundary Finite Element Method (SBFEM) emerged as an efficient and accurate strategy where only the element's skeleton is discretized, and the shape functions are defined using a semi-analytical approach [1]. The SBFEM approximations are akin to the traditional H^1 approximation and do not satisfy the divergence-free condition by construction.

In this work, we propose to extend essential ideas of SBFEM to mixed finite element approximations. The Hybridized-Mixed technique is applied to infinitesimal finite cells [2] in order to obtain the SBFEM coefficient matrices. These matrices represent the known Riccati ODE, and its solution provides the shape functions for locally conservative mixed finite elements. Thus, an SBFEM-H(div) function space is constructed to approximate the flux, and a discontinuous SBFEM space is defined for the pressure.

The mathematical formulation proposed in this study was implemented in an object-oriented FE library. Numerical tests of a Darcy flow in a 2D domain were performed and rates of convergence were computed. We also considered domains including square-root singularities, depicting the capacity of the method for simulating a flow in a fractured porous media. Optimal rates of convergence were observed, including for the flux and high-order approximations, illustrating the accuracy of the proposed approach.

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Quadrilateral Scaled Boundary Spectral Shell Elements with Assumed Natural Strains

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Key Words: *Scaled Boundary Finite Element Method, Shell Element, Spectral Element, Assumed Natural Strain Method, Locking*

We construct within the framework of the scaled boundary finite element method [1,2] new variable-order shell elements that require only the shell midsurface to be discretized, contain no rotational degree of freedom and adopt the full three-dimensional constitutive relationship. In the formulation, a shell element is treated as a three-dimensional continuum undergoing small deformations and its middle surface is represented via a quadrilateral spectral element. The entire shell geometry is described through normal scaling of the middle surface and the displacement field across the thickness is expressed approximately by interpolating the displacements on the top, middle and bottom surfaces with quadratic Lagrange shape functions. The assumed natural strain method is applied to eliminate transverse shear locking, membrane locking and curvature thickness locking while the volumetric locking is alleviated by elevating the polynomial order. Numerical examples demonstrate that the developed shell elements are superior in applicability, accuracy and efficiency.

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Resolving quasi-brittle fractures in anisotropic domains with SBFEM

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Key Words: SBFEM, phase field, quasi-brittle fracture, anisotropy

The Scaled Boundary Finite Element Method (SBFEM) has emerged as a promising alternative to standard discretization approaches that attempts to fuse the advantageous characteristics of the Finite Element Method and Boundary Element Method onto one computational framework. Similar to the BEM, only the boundary of the domain is discretized hence reducing the dimensionality of the problem by one. The method becomes attractive especially for the case of phase field fracture simulations where fine mesh resolutions are typically required. Contrary to the BEM, no fundamental solution is required, and the overall scheme relies solely on an ansatz, as in the standard FEM. The case of brittle fracture in isotropic domains was very recently treated using SBFEM in [1].

In this work, we develop a framework for the simulation of fractures propagating in quasi-brittle anisotropic domains using the 3-parameter cohesive phase field model for anisotropic media proposed in [2]. The SBFEM is employed to discretize both the phase field and displacement based equilibrium equations of the problem. A staggered solution strategy is employed, and the solution is performed over quad-tree meshes that facilitate adaptive mesh refinement. The accuracy and efficiency of the method as compared to the standard FEM is investigated through a set of benchmarks. Furthermore, the sensitivity of the method vis-à-vis the mesh quality is examined. Our preliminary results demonstrate that the SBFEM results in robust and well behaved and accurate solutions.

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SBFEM for hydrodynamic problems with cavitation

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Key Words: Scaled Boundary Finite Element Method, Reynolds Equation, Hydrodynamic Bearing, Cavitation, Elrod Algorithm, Rotordynamics

Hydrodynamic bearings are employed because of their high load support and damping capacity, their durability, and their compact design. However, in high-speed rotor systems, the nonlinear fluid-structure interaction can cause self-excited vibrations leading to noise emission, wear, and a reduced energy efficiency. Transient rotordynamic simulations offer a valuable tool for the prediction of this behavior but are often time-consuming, since the computation of the bearing forces requires a solution of the Reynolds equation in every time step. This equation is usually solved by means of look-up tables or numerical methods, but in both cases, a tradeoff between accuracy and computational efficiency is necessary.

In a recent study [1], a semi-analytical solution of the Reynolds equation based on the Scaled Boundary Finite Element Method (SBFEM) [2] has been developed with the objective of reducing the numerical effort of rotordynamic simulations. This solution is now extended to consider cavitation, which is a physical effect often incorporated into numerical models for improving the accuracy of the simulation. When the hydrodynamic pressure falls below a threshold, gas cavities occur inside the lubricant, changing the fluid properties and affecting the pressure generation. This effect is described by cavitation models such as the Elrod algorithm [3], which is used in this study. The corresponding SBFEM formulation of the Reynolds equation is derived, and exemplary bearing simulations are performed. It is observed that the numerical stability of the developed solution as well as the accuracy of the resulting bearing forces depend substantially on the attitude angle of the shaft relative to the position of the oil supply groove. This is due to a simplification necessary in the SBFEM model, namely that the boundary between the cavitation zone and the pressure zone has to be parallel to the scaling direction (the analytically treated coordinate direction). Possible strategies for overcoming this disadvantage are discussed in this contribution.

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Simulation study on meso-level concrete cracking based on SBFEM method considering the influence of cohesion

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Key Words: *Concrete micromechanics; SBFEM; Quadtree mesh; crack propagation; stress intensity factor; cohesive interface elements.*

Abstract：The method by combining SBFEM and Quadtree mesh is developed for analyzing the interface crack problems of double material plate. The distributions of generalized stress intensity factors can be obtained around crack tip within 360 degrees. According to the distribution rules of the generalized stress intensity factors, the cracking criterion with considering the comprehensive effect of K is proposed. The influence of the size of the crack tip element on the singular order is discussed and the reasonable size of crack tip element for fracture analysis is proposed. Nonlinear cohesive interface elements with normal and shear traction-separation constitutive laws are considered in the cracking process. The effect of hydraulic fracturing on the concrete cracking and propagation at mesoscale is discussed. The methods combining SBFEM and Quadtree mesh are used for numerical analysis of concrete specimens at mesoscale with considering the interaction between the water pressure along crack surface and the crack propagation. The finite volume method is used to establish the coupling model of water pressure along crack surface and crack width. The water pressure distribution along crack surface is solved iteratively. The modelled crack paths and load-carrying capacities of concrete specimens are in excellent agreement with the experimental data.

Spatially Variable Coal Slope Stability Analysis using Image-Based Scaled Boundary Finite Element Method

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Key Words: *Slope stability, SBFEM, spatial variation, image-based meshing*

Slope stability analysis is a challenging task when complex stratigraphies, complex geometries and spatially variably soil parameters are considered. Numerical methods, such as the finite element method are commonly used in slope stability analyses, however these methods require significant user input when meshing geometries consisting of heterogeneous and spatially variable materials. This paper presents a numerical technique combining the scaled boundary finite element method and image-based meshing for slope stability analysis. The inputs for the analyses require images detailing the strata and the spatial variation of the material properties within the strata. Quadtree decomposition was applied to simultaneously generate meshes and consider the spatial variation of material properties directly from the images through a mapping technique. The stability of slopes were analysed assuming an elasto-plastic Mohr-Coulomb constitutive model for the soil. The shear strength reduction technique is applied to evaluate the shear reduction factor iteratively to define the factor of safety of the stable slope. Coal slope at Yallourn open-pit mine,Victorial, Australia was used as a case study to demonstrate the application of the presented method.

Three-dimensional Non-linear Numerical Analysis of Randomly Distributed Short Fiber-Reinforced Composites using the Scaled Boundary Finite Element Method

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Key Words: *Scale boundary finite element method, Short fiber-reinforced composite, Non-linearity, Discrete modelling, Fiber/matrix debonding*

This contribution presents the three-dimensional numerical modelling of randomly distributed short fiber-reinforced composites (SFRCs) with the scaled boundary finite element method (SBFEM)[1]. Automatic mesh generation of SFRCs in a discrete fashion is utilized to generate conforming meshes of the matrix and the fibers[2, 3]. To this end, three phase non-linear materials including matrix, fiber and interface are incorporated, which allows to simulate the progressive failure of SFRCs considering matrix cracking, fiber breakage and fiber/matrix debonding simultaneously. The analyses are performed on the platform ABAQUS through polyhedral user elements (UEL) derived by the SBFEM[4]. Damage constitutive law is employed to simulate the non-linear behaviour of matrix. The fiber and interface are represented by beam and spring elements with inelastic mechanical properties, respectively. The proposed model provides a relatively realistic simulation of randomly distributed SFRCs which considers complex microstructures with less demanding of computational resources and human efforts on meshing. The accuracy, robustness and efficiency of the proposed approach are demonstrated by means of serval numerical examples.

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Time integration methods for wave propagation modeling in unbounded domains using the scaled boundary finite element method

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Key Words: Scaled Boundary Finite Element Method, Wave Propagation, Unbounded Domain, Explicit Dynamics

To solve wave propagation problems in soil or soil-structure domains using standard finite elements, very large domains must be modeled to avoid reflections at the artificial boundaries or to increase the accuracy of absorbing boundary conditions. Especially for three-dimensional problems, this procedure can become very costly and inefficient.

An alternative approach is to use the scaled boundary finite element method (SBFEM) and to define an unbounded subdomain, which is described by scaling the soil-structure interface towards infinity. Here, the reaction forces at this interface are calculated by using the acceleration unit-impulse response method. As a result, a convolution integral is present in the equations of motion of the bounded domain. In existing publications, these are solved using implicit time-stepping schemes, such as Newmark's method [1].

In this contribution, an explicit time integration scheme for acceleration unit-impulse response-based models of unbounded soil-structure systems is proposed. The motivation is that various techniques for increasing the efficiency of bounded domain models, such as mass lumping [2] or exploiting similarity of structured meshes together with parallel computing [3], are tailored to explicit solvers. This can be exploited especially in large three-dimensional models and reduce computation time. Both strategies, implicit and explicit methods, are compared and discussed with respect to benefits and disadvantages in the context of transient soil-structure interaction modeling.

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A Virtual Element Method to resolve ductile fractures in particulate composites with arbitrary shaped inclusions

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Key Words: VEM, phase field, ductile fracture, cohesive surfaces, particulate composites

Particulate composites are widely used in the aerospace, automotive, and construction industry to improve the mechanical performance of structural components. Additive manufacturing paved the way for generating tailor made multi-material layouts of optimal properties; unfortunately, optimum additively manufactured domains often involve tessellated geometries. This gives rise to complex and involved damage patterns that need to be accurately estimated at the design phase. This necessitates the use of numerical methods, e.g. the FEM to resolve damage patterns. However, when the domain comprises arbitrarily shaped inclusions the efficiency of the solution procedure is hindered by the mesh refinement restrictions imposed by the domain topology.

Polygonal element topologies have been shown to provide flexibility to overcome such issues.The Virtual Element Method [1] emerged from Mimetic Finite Differences (MFDs) as an accurate and efficient alternative to FEM, designed to address this issue. Shape functions are implicitly defined through carefully chosen degrees of freedom. State matrices are computed through projection maps without affecting optimal error convergence rates. In this work, we explore the potential of the VEM to efficiently resolve ductile fractures in particulate composites within a small strain setting. Driven by the work of [2] we develop a ductile fracture phase field model within a VEM setting and combine it with a cohesive surface approach to account for de-bonding at the matrix to inclusion interface. Further to the current state-of-the-art, the case of J2 and Druger-Prager plasticity is examined, accounting for metal and ceramic matrix composites, respectively.

Our preliminary results demonstrate that the VEM results in robust solutions that are more computationally efficient when compared to the standard FEM while achieving in resolving fractures in matrices containing arbitrary shaped inclusions when compared to the standard Finite Element Method.

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Adaptive Mesh Refinement Procedures for the Virtual Element Method

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Key Words: *Virtual element method, adaptive mesh refinement*

The virtual element method (VEM) is an extension of the finite element method that permits arbitrary polygonal element geometry in two dimensions [1]. This mesh flexibility means that the VEM is well-suited to problems involving adaptive mesh refinement. However, the virtual element function spaces are defined such that quantities are only explicitly known on element edges. Thus, the well-known approaches to mesh adaptivity developed for finite elements cannot be directly applied to problems involving the VEM.

A variety of approaches to adaptive mesh refinement procedures have been formulated and implemented for the VEM for the case of two-dimensional elastic problems. The approaches are motivated by seeking to improve the approximations of the displacement and/or strain fields. The performance of these approaches has been investigated in terms of accuracy vs computational cost compared to a traditional reference mesh refinement procedure.
The performance was studied through a range of numerical benchmark problems, including the well-known L-shaped domain and punch problems.

The the results demonstrate that each of the adaptive mesh refinement procedures consistently generates solutions of equivalent accuracy to the reference procedure while using significantly fewer degrees of freedom, and significantly less run time, representing a dramatic improvement in computational efficiency and improved convergence behaviour [2].

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Adaptive Virtual Element Method

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Key Words: Polytopal meshes, Virtual Element Method, Adaptivity

Virtual element method (VEM) is a relatively new discretization paradigm which allows the numerical solution of partial differential equations on general polytopal meshes. This geometric flexibility is very useful in many solid and fluid mechanics applications, in particular when adaptive mesh refinement is employed on moving or very complicated geometries. In this talk, we present recent advancements in the understanding and practice of the adaptive virtual element method (AVEM) for the solution of partial differential equations. In particular, we will discuss through extensive numerical experiments both practical and theoretical issues, ranging from the strategy of refining a general polytopal to the study of the convergence and computational complexity of the adaptive algorithm based on the iteration of the classical paradigm:

$$\texttt{ESTIMATE} \rightarrow \texttt{MARK} \rightarrow \texttt{REFINE} \rightarrow \texttt{SOLVE}$$

where the module `ESTIMATE` computes a posteriori error estimators, `MARK` identifies the polytopal elements to be refined, `REFINE` performs the refinement of the marked elements and `SOLVE` finds the discrete approximation on the adaptively refined mesh.

First-Order Virtual Elements for the Shear Deformable Plate Problem

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Key Words: *Reissner-Mindlin plates, Virtual Element Method, Locking-free, Polygonal meshes*

In this contribution, the construction of first-order virtual elements for the shear deformable plate problem is presented and discussed. Transverse displacement and rotations are assumed as independent variables, in the framework of a standard displacement-based variational formulation. A piecewise linear approximation is adopted on the boundary of the polygonal element for both transverse displacement and rotations.

Uncoupled polynomial approximations for the generalized strains, with different polynomial degrees for the bending and shear parts, are assumed for the construction of the consistent term of the stiffness matrix.

With the aim of preventing shear locking in the thin-plate limit and keeping the construction of the element as simple as possible, an indirect enrichment of the approximation of the transverse displacement with respect to that of the rotations is introduced through a selective scheme for the stabilization term of the stiffness matrix [1].

The performance of the method is tested through several numerical examples involving thin and thick plates and by using different polygonal meshes. As a result, the proposed first-order virtual elements allow to save degrees of freedom with respect to existing approaches [2,3] while keeping comparable results.

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Virtual Element Method (VEM)-based 2D Cohesive Fracture Simulation with Element Split and Stress Recovery

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Key Words: *Virtual Element Method, Cohesive Fracture, Element Split, Stress Recovery*

This study presents a computational framework for mixed-mode cohesive fracture simulation using the virtual element method (VEM). Because VEM is able to consistently handle arbitrary shped elements [1], VEM is one of the best candidates for the crack path representation in cohesive fracture simulation. To represent an arbitrary and curved crack path on polygonal discretization, the element splitting approach is employed [2,3]. For the accurate approximation of a crack-tip stress field and the crack propagation direction, the virtual grid-based stress recovery scheme (VGSR) [3,4] is utilized with the maximum strain energy release rate. To verify and validate the accuracy and robustness of the proposed computational framework, the mixed-mode fracture examples are illustrated. Numerical results demonstrate that VGSR-based crack growth criterion well captures an accurate crack path direction, even under the biaxial stress state. In addition, the computed crack patterns using the element splitting process show that smooth and curved cracks on polygonal elements, and good agreement with the experimental results.

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Virtual Element Method for Large Deformations of Plates with Isometry Constraints

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Key Words: Virtual element method, Nonlinear plates, Γ-convergence, Discrete gradient flow

In this presentation, we introduce an ongoing work about a virtual element method (VEM) for approximating large deformations of plates with isometry constraints. We study both single layer plates and bilayer plates in this project, and for latter we consider both Dirichlet boundary conditions and free boundary conditions. The problem consists of minimizing a bending energy subject to a nonlinear and nonconvex constraint. The energy is discretized using VEM and a discrete gradient flow is designed for computing discrete minimizers. We first show Γ-convergence of the discrete energy to the continuous one. Then we prove that the discrete gradient flow decreases the energy at each step and computes discrete minimizers with control of the isometry constraint defect in L^∞ norm. We also illustrate the performance of our algorithm with several insightful simulations.

Contrary to previous finite element methods (FEM) for this type of problem, which use Kirchhoff elements [1], discontinuous Galerkin (DG) methods [2] and local discontinuous Galerkin (LDG) methods [3], this VEM method can formally allow arbitrary order of discretization, and this is a main advantage of the our method. A key ingredient in the analysis is an inverse inequality for L^∞ norm of functions in a virtual element space. Moreover, in the method for bilayer plates, we also propose a novel enhanced virtual element space and interpolation operator, which turns out to be crucial in the treatment of the nonlinear term appearing in the energy for bilayer plates.

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Boundary Variation Diminishing scheme using β-variable THINC scheme for compressible multiphase flow

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Key Words: *Finite volume method, High-order and shock-capturing scheme, BVD principle*

Boundary Variation Diminishing (BVD) schemes [1] have been recently developed as a high-fidelity Godunov-type finite-volume method for compressible flows. In general, it is necessary to reduce numerical dissipation of the numerical schemes in order to resolve wide-range scales of flow structures. The numerical dissipation can be effectively reduced by the BVD principle [1] that diminishes the difference between the left- and right-value of a reconstructed physical quantity at the cell boundary. Following this principle, the BVD scheme was extended to combine the existing high-order scheme with the THINC (Tangent of Hyperbola for INterface Capturing) scheme [2] that is suitable for capturing the discontinuities. Such hybrid-type schemes can resolve both smooth and discontinuous solutions with high resolution.

To explore further possibility of the BVD schemes, we investigate the effectiveness of β-variable THINC scheme [3], in which the steepness parameter β of the THINC function is changed locally. The algorithm to calculate the appropriate value of β for each cell is developed and the β-variable THINC scheme is embedded into the existing BVD formulation. The new BVD scheme can resolve the small vortices more clearly by adapting the value of β based on the local solution and simultaneously suppress the computational cost by reducing the number of candidate reconstruction functions.

Furthermore, the BVD principle can be applied to the calculations of the compressible multi-phase flows including moving interfaces as in cavitation and atomization. In such flows, the shape of the gas-liquid interface may change drastically. Therefore, it is more important than in the case of single-phase flows to suppress the numerical dissipation and capture the discontinuous solutions with high resolution. The effectiveness of the BVD scheme will be assessed by the benchmark tests relevant to actual problems (primary breakup of liquid jet inside rocket engine combustors, etc.).

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Efficient approaches to CFD simulations of reactive flow using reliable chemical reaction models

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Key Words: *Combustion, Chemical Reaction, Stiffness*

Combustion has been applied as an energy source in various fields, but its detailed phenomena are still unknown due to the complex interaction of fluid dynamics and chemical reactions. Therefore, it is desirable to reproduce combustion phenomena by CFD simulation. However, the scale of a practical combustor is much larger than that of a flame and solving chemical reactions with an increasing number of strongly nonlinear equations to be solved dramatically increases the computational cost. For this reason, CFD simulations of combustion often solve chemical reactions in a greatly simplified manner, which does not lead to a detailed understanding of combustion phenomena. In addition, there is a recent need to reduce CO_2 emissions. Therefore, there is a rapid demand for the development of combustors that can operate near the combustion limit to achieve higher efficiency and the use of biofuels and synthetic fuels, and it is becoming difficult to deal with this issue using conventional CFD simulations that cannot handle chemical reactions accurately.

The main computational cost is due to the chemical reactions, for which implicit methods are generally applied due to their stiffness. As a result, the computational cost of generating the Jacobi matrix used in implicit methods is the square or cube of the number of chemical species. In the case of hydrocarbon fuels, the number of chemical species ranges from hundreds to thousands, making the computational cost impractical. Accordingly, Morii et al. have developed robust integration methods that do not require the Jacobi matrix [1, 2]. With the development of these methods, the computational cost is only proportional to the number of chemical species, and the computational cost has been significantly reduced. To further reduce computational cost, the developed methods have been incorporated into PeleC software [3], which incorporates AMReX, a library of adaptive mesh refinement methods. As a result, direct numerical simulations on an experimental scale are now possible and the results can be compared quantitatively with respect to knocking [4], which has been a problem in improving the efficiency of SI engines. However, in order to apply CFD simulation to the development of actual engines, further reduction of the computational cost is required.

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GPU Accelerated Paired Explicit Runge-Kutta Schemes in HORUS

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Key Words: GPU, accelerated, high-order, paried explicit Runge-Kutta, speedup

Scale resolving simulations, such as Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS), require accurate, efficient, and stable discretizations of the Navier-Stokes equations. Recent research has demonstrated that high-order spatial discretizations, such as the Flux Reconstruction (FR) approach, are particularly appealing when coupled with explicit Runge-Kutta (RK) schemes on Graphical Processing Units (GPUs). This has been shown to be an order of magnitude faster and, simultaneously, an order of magnitude more accurate than industry standard Finite Volume (FV) methods [1]. However, one disadvantage is that high-order schemes have increased numerical stiffness. This limits the maximum allowable time step size, and prohibits their use beyond Reynolds numbers of approximately $Re \leq 10^6$.

Paired Explicit RK (P-ERK) schemes have been proposed as a solution to this problem [2]. Families of P-ERK schemes have an arbitrary number of stages, and each member of a family has a different number of *active stages*. Members with more active stages require more unsteady residual calculations, yielding larger stability limits. Members with fewer active stages require fewer unsteady residual calculations, but have lower computational cost. All members from the same family can be paired seamlessly, allowing schemes with more active stages to be used in stiff regions, wheras schemes with few active stages are used in non-stiff regions. Previously, it has been demonstrated that P-ERK schemes yield 5-10x speedup relative to classical explicit RK methods on Central Processing Units (CPUs).

In this work we will demonstrate the utility of P-ERK schemes combined with GPU acceleration in the High-ORder Unstructured Solver (HORUS) developed at Concordia University. Using this approach HORUS can obtain speedup factors in excess of 30-50x on a per-node basis when compared to classical RK schemes on CPUs. This is observed over a range of different simulations including turbulent flow over a sphere, tandem spheres, and a stalled airfoil. In this talk we will discuss implementation details of P-ERK schemes on GPUs, partitioning, scaling, and show results for a range of different practical LES/DNS simulations. Finally, recommendations will be made for the use of P-ERK schemes combined with high-order methods for high Reynolds number flows.

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Hybridized Flux Reconstruction Methods for Convection-Diffusion Problems

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Key Words: Flux Reconstruction, Implicit Discretizations, Hybridization, Convection-Diffusion problems

High-order methods have become a promising approach for the analysis and optimization of problems involving complex fluid flows. In particular, the flux reconstruction (FR) method of Huynh [2] has been shown to be an attractive choice amongst a variety of existing schemes [3]. The FR approach is able to recover existing high-order discretizations and define new methods via the choice of correction functions [2, 4].

Often, high-order methods are used in conjunction with explicit time-stepping due to their simplicity. However, for stiff problems, the maximum allowable time-step size can be prohibitively small. On the other hand, implicit time-stepping is also prohibitively expensive due to a large number of degrees of freedom in the resulting systems of equations. These scale as p^{2d} where d denotes the number of dimensions.

In this work, we propose a new implicit flux reconstruction framework for convection-diffusion problems. These methods apply the hybridizable high-order discontinuous Galerkin approach of Cockburn et al. [1] to the family of FR schemes. This hybridization allows for a reduction of the scaling of the implicit system size to that of an effective lower dimension. This is possible by introducing unknowns on the skeleton of the grid as well as an additional global conservation statement. Hence, the problem can be rewritten in terms of this trace unknown using static condensation.

We will show how hybridized FR methods can significantly reduce the computational cost of convection-diffusion implicit problems, particularly for higher-order discretizations. Furthermore, we present a new elementwise postprocessing scheme in which we use FR correction functions to improve flux convergence and thus obtain solutions that are more accurate and have better convergence rates. These findings are supported by verification and validation studies on a series of numerical examples.

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INVESTIGATION ON GRID RESOLUTION REQUIREMENTS FOR HIGH-ORDER IMPLICIT LARGE EDDY SIMULATION

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Key Words: Optimal Grid Resolution, Implicit Large-Eddy Simulation, Discontinuous Galerkin Method, High-order Method, Turbulent Flow, Kriging Meta-model

This research aims to find a baseline grid configuration that provides cost-efficient and accurate solutions for high-order implicit large-eddy simulation (ILES). To achieve this, the optimal grid resolution for high-order ILES is estimated using the Kriging meta-model. Based on the Kriging optimization, approximated relational expressions between the solution approximation order and the optimal grid configuration, named the grid-$\mathbb{P}^k$ relations, are proposed in order to provide a guideline of a proper grid resolution for ILES using high-order methods.

A fully developed turbulent channel flow at $\mathrm{Re}_\tau = 180$ is employed as a model problem to elicit the optimal grid resolution. Every computation is conducted using a high-order accurate solver based on the modal Discontinuous Galerkin method [1]. Turbulent statistics are collected from the turbulent channel flow simulation on a series of grid configurations (i.e., minimum wall-normal grid spacing, stretch ratio, and spanwise grid spacing). An objective function is defined as the L_2 error of the streamwise mean velocity, and a cost constraint is imposed to avoid a trivial conclusion. Through the optimization process by the Kriging meta-model and genetic algorithm, a set of optimal grid resolutions for various solution approximation orders (*P2*, *P3*, and *P4*) are obtained.

From the optimization results, the grid-$\mathbb{P}^k$ relations estimating the optimal grid resolution for high-order ILES are proposed. Those are validated by turbulent channel flows at $\mathrm{Re}_\tau = 180$, $\mathrm{Re}_\tau = 395$, and $\mathrm{Re}_\tau = 550$ and external transitional flows over an SD7003 airfoil at $\mathrm{Re} = 60,000$. The ILES results of turbulent channel flows are compared to DNS results, and the flow over the SD7003 airfoil is compared to other high-fidelity computations. As a result, the computations of both internal and external flows match well with the reference solutions so that support the validity of the proposed grid-$\mathbb{P}^k$ relation.

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Large-Eddy Simulations of Supercritical Jet Flames by Flux-Reconstruction Method with Invariant-Region-Preserving Limiter

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Key Words: *Flux Reconstruction, Supercritical Jet, Non-premixed Flame, LES*

Modern high performance liquid rocket engines (LREs) operate at very high combustion pressures over 10 MPa with propellant injection at cryogenic temperatures. Under such trans-critical conditions, the real-gas effect of propellants must be considered to predict liquidlike dense fluid behaviour and nonideality of thermodynamic properties [1]. The large and abrupt change of thermodynamic properties across the contact discontinuity between cryogenic propellants and hot combustion gas make robust and accurate simulations difficult. In particular, the high-order schemes required for accurate large-eddy simulations (LES) are more likely to suffer from numerical instability.

In this study, the high-order flux reconstruction (FR) method [2] is developed for liquid oxygen (LOX) and gaseous hydrogen (GH2) coaxial jet flames under supercritical pressures. The SRK equation of state is used to account for real-gas effect and the Chung's transport coefficient model is employed for LOX. To overcome the numerical instability for the conservative FR formulation, the invariant region preserving (IRP) limiter [3] is extended for the real-gas mixture. First, two-dimensional LOX/GH2 inert turbulent mixing layer is computed for verifying the performance of the proposed scheme. Then, LES of the turbulent diffusion flame of single coaxial LOX/GH2 injector is performed using the flamelet progress-variable (FPV) tabulated approach [4]. A high-performance computing application of the full-scale engine combustor LES with more than 500 injectors will be presented.

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On the Use of Entropy Stable Flux Reconstruction for Large Eddy Simulation

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Key Words: *Entropy stable flux reconstruction, Large-eddy simulation*

High-order numerical methods, such as Discontinuous Galerkin (DG) and Flux Reconstruction (FR), i.e. FR-type methods, are particularly appealing for the Large Eddy Simulation (LES) of turbulent flows, as they show significant potential to improve simulation accuracy at comparable or reduced computational cost [1]. In LES, the unsteady turbulent motion is decomposed into a filtered (resolved) component, representing large-scale energy containing eddies, and a residual component by use of a low-pass filter. Due to the convenient spectral dissipation properties of FR-type methods, this filtering can be performed implicitly by the numerical dissipation of the spatial discretization scheme; this is referred to as implicit LES (ILES). Furthermore, in LES, the effect of the residual motions on the resolved scales is modelled by a sub-grid scale (SGS) model, representing a residual-stress tensor; which effectively dissipates turbulent kinetic energy (TKE) from the smallest resolved scales. In general, the truncation error of FR-type schemes resembles an additional numerical stress and amounts to an implicit SGS model, having similar influence as conventional SGS models; this is referred to as no-model ILES. However, despite the success of FR-type methods for the no-model ILES of turbulent flows at moderate Reynolds number flows, their application to industrially relevant simulations, consisting of higher Reynolds number flows or requiring coarser grids, has been limited ultimately due to the absence of nonlinear stability. It has recently been demonstrated that these limitations can be overcome with the use of energy stable DG schemes for ILES, possessing superior robustness and the ability to strongly increase fidelity on very coarse grids [2]. These promising results encourage the development of provably nonlinearly stable FR schemes for ILES, given the advantages of FR over DG such as larger explicit time stepping. Recently, the first critical step towards this has been taken with the newly proposed framework of generalized provably nonlinearly stable FR schemes in split form that enable both energy/entropy stability and conservation proofs, referred to as Entropy Stable Flux Reconstruction (ESFR) [3]. In this work, we present a novel ILES approach based on adaptive nonlinearly stable ESFR schemes (ESFR-ILES) that is well suited for shock-free turbulent flows by extending the original work on ESFR schemes to 3D systems of conservation laws. The use of the ESFR schemes for the ILES of shock-free turbulent flows is investigated and its performance with the use of various SGS models is demonstrated for both the viscous Taylor-Green Vortex (TGV) problem, and a decaying homogeneous isotropic turbulence (DHIT) test case.

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Optimization of Non-Conventional Airfoils for Martian Rotorcraft using Direct Numerical Simulations

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Key Words: Martian Aerodynamics, Optimization, Direct Numerical Simulations, Low-Reynolds-Number

Martian atmospheric conditions present various challenges when designing rotorcraft. Specifically, Mars has a thin atmosphere with lower pressure and density compared to Earth, reducing the performance of conventional airfoils. Additionally, the speed of sound on Mars is approximately 72% of that on Earth which constrains rotor speeds in order to avoid high Mach numbers at rotor blade tips. These unique conditions require Martian rotor blades to operate in a low-Reynolds-number ($\approx 10^3$ to 10^4) compressible flow regime, for which conventional airfoils have not been designed.

Recent studeis have investigated the perfromacne of non-conventional airfoil designs, with sharp edges and flat surfaces, under Martian atmospheric conditions [1] [2]. Further studies have explored optimizing such airfoils using Genetic Algorithms (GAs) [2]. These involve a high number of cost function evaluations, and hence typically Reynolds-Averaged Navier Stokes (RANS) solvers are employed to bound overall cost. However, RANS solvers have reduced predictive capability when the flow becomes unsteady at moderate angles of attack, thus limiting the utility of the approach. Our work looks to overcome this limitation by undertaking optimization using high-order Direct Numerical Simulations (DNS) using PyFR (www.pyfr.org) [3].

In this talk, we will present results from GA based multi-objective optimizations of non-conventional airfoils at various angles of attack under Martian atmospheric conditions. The findings can be used to help design new rotorblades for next-generation Martian rotorcraft.

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PyFR: Latest Developments and Future Roadmap

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Key Words: High-Order Methods, Fluid Dynamics, Direct Numerical Simulations

PyFR is a high-order accurate Computational Fluid Dynamics (CFD) solver based on the Flux Reconstruction approach of Huynh [1]. It is written in Python, and can target a range of hardware platforms via an innovative Mako-based domain specific language [2]. Over the past decade PyFR has matured into an established part of the open source CFD ecosystem. It now has an active community of users around the world, and is routinely applied to undertake high-fidelity scale-resolving simulations across a range of application areas, including at extreme scale. This talk will present results from some of the latest simulations to be undertaken with PyFR, and provide insight into some of our latest technological developments, including cache blocking optimisations for the CPU backend, turbulence injection approaches, and new shock capturing methods. Finally, we will outline our roadmap for future development of the solver.

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Third-Order Paired Explicit Runge-Kutta Schemes for Stiff Systems of Equations

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Key Words: *Runge-Kutta methods, Optimal time-stepping, Flux reconstructions*

In this paper, we expand the family of Paired Explicit Runge-Kutta methods, referred to as P-ERK schemes, to third-order accuracy in time. The P-ERK approach is particularly appealing for the solution of locally stiff systems of Partial Differential Equations (PDEs) to reduce computational cost. Previously, it was shown that P-ERK family members with different numbers of derivative evaluations can be applied to different regions of the domain, based on local stiffness requirements, so the global time-step to be taken as large as possible [1]. However, the original family of P-ERK schemes is limited to second-order accuracy [1]. In this study, we introduce a new family of P-ERK methods with third-order accuracy, and optimize them specifically for high-order flux reconstruction [2] spatial discretizations [3]. We verify that these methods achieve their designed order of accuracy for an isentropic vortex case with arbitrary combinations of schemes. We then demonstrate that simulations with the third-order P-ERK family can achieve significant speedup factors compared with classical third-order Runge-Kutta methods. These speedup factors are obtained for laminar and turbulent flow over an SD7003 airfoil and a turbulent tandem spheres simulations. These results demonstrate the P-ERK schemes are a suitable approach for accelerating high-order accurate simulations of unsteady turbulent flows.

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Utilizing Time-Reversibility for Shock Capturing in Nonlinear Hyperbolic Conservation Laws

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Key Words: *Shock capturing, artificial viscosity, hyperbolic systems*

The approximation of systems of nonlinear hyperbolic conservation laws remains a challenge for the development of many high-resolution numerical schemes due to their lack of robustness in the vicinity of discontinuities. For these systems, discontinuities can, and often do, arise from initially-smooth data, and without proper treatment, can result in spurious oscillations that can degrade the quality of the solution or cause the scheme to fail altogether. Various nonlinear stabilization techniques have emerged among practitioners of high-order numerical schemes, and these techniques share a common goal of robustly resolving discontinuous features while recovering high-order accuracy in smooth regions. The addition of an artificial viscosity can be considered to be the most ubiquitous stabilization method for numerical schemes. This approach possesses several favorable properties in that it can robustly resolve discontinuities, is simple to implement and extend to unstructured grids, and has rigorous mathematical backing in the context of hyperbolic conservation laws. However, determining where and how much artificial dissipation to apply is an open problem, as the stability of the scheme can suffer if not enough dissipation is introduced in the vicinity of a shock, but solution accuracy in smooth regions can be severely degraded if unnecessary dissipation is applied.

In this talk, we will describe a novel approach for estimating the artificial dissipation required for robustly resolving discontinuous features in hyperbolic conservation laws. The artificial viscosity term is calculated based on an estimation of the reversibility of the system, utilizing the fact that entropy production by shocks imposes a time-irreversibility condition on the solution. The proposed approach can be applied without any additional governing equations, is independent of the mesh and approximation order, does not require a priori knowledge of the hyperbolic system in question, and requires the use of only one tunable parameter. The primary novelty of this method is that the resulting artificial viscosity is unique for each component of the conservation law which can significantly improve the accuracy of the approximation of systems in which some components exhibit discontinuities while others do not without additional computational cost. The efficacy of this method will be shown through numerical simulations in the context of a high-order discontinuous spectral element method for hyperbolic conservation laws such as the Euler equations and ideal magnetohydrodynamics.

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A High-Order Extended Discontinuous Galerkin Method for Coupled Multi-Material Sharp Interface Problems

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Key Words: Unfitted, Cut-cell, Immersed, Sharp interface, High-order, Discontinuous Galerkin

A wide range of multiphysics problems arising from different scientific fields are dominated by multi-material interactions. When complex interface geometries are at stake, the applicability of established boundary or interface mesh-conforming discretization may be strongly limited, especially for moving interface problems. Past and current intense developments of geometrically unfitted methods have opened the way to new simulations capabilities. Among this broad family of methods, the so-called eXtended Discontinuous Galerkin (XDG) Method introduced in [1] and further developed in our previous work [2, 3] is the focus of the present paper.

While highly increasing versatility, decoupling the finite element approximation space from the background mesh entails additional difficulties for the XDG method that will be addressed in this work: (i) interface representation and motion, (ii) management of independent sets of degrees of freedom in cut-cells, (iii) integration over implicitly defined domains, (iv) treatment of small cut-cells, (v) time-integration on moving domains, (vi) interface coupling conditions enforcement.

The presentation will cover the aspects described above accompanied by illustrative test cases. Particular emphasis will be placed on the novel proposed coupling strategy for complex multi-material problems, such as viscous compressible gas-liquid flows.

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A higher-order fictitious domain method for structural membranes and shells

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Key Words: *Membranes, Shells, Cut FEM, Trace FEM, fictitious domain method, PDEs on manifolds.*

Structural membranes and shells are modelled by partial differential equations posed over curved two-dimensional surfaces in the three-dimensional space. Herein, these surfaces are embedded in a three-dimensional background mesh composed by higher-order elements and a fictitious domain method (FDM) is proposed for the approximation. Such a method may also be labelled Cut FEM or Trace FEM [3,4]. The governing equations of structural membranes featuring large displacements as well as linear Kirchhoff-Love and Reissner-Mindlin shells are formulated based on the Tangential Differential Calculus (TDC) [1-3]. The geometries of the structures are implied by the level-set method, prescribed at the nodes of the higher-order background mesh and interpolated in-between.

In any FDM, the following three issues have to be addressed: (1) The numerical integration of the weak form in the (three-dimensional) background elements which are cut by the membrane or shell. Therefore, the zero-level sets of the level-set functions have to be identified and integration points defined. (2) The application of boundary conditions within the background elements which is done based on Nitsche's method here. (3) The stabilization with respect to shape functions with extremely small supports on the structure. When using FDMs for the approximation of PDEs on manifolds, a stabilization is also required to tackle linear dependencies of the three-dimensional shape functions of the background mesh when applied to the analysis of the (curved) two-dimensional structures. Numerical results show the success of the proposed formulation.

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A Poisson problem with internal Dirichlet condition motivated by geophysical applications

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Key Words: Geophysics, Parametric problems, Inverse problem, Poisson problem, Interface

Inverse problems in geophysics seeking to understand the current state of planet Earth use data from multiple observables and involve a variety of physical principles. One of the key fields to determine is the temperature, and it affects almost all the other physical quantities involved (e.g. densities, viscosities, wave propagation velocities, among others).

Within inverse problems, the parameters determining the interface locations are usually to be determined. Some of these interfaces are defined by isotherms. The inverse solver requires the solution of many forward problems where the location of the interface change. Consequently, the isotherm position in the computational domain changes. Setting Dirichlet conditions within the domain might lead to ill-posed problems.

In this work, we will analyse the one, two and three-dimensional cases in a simple setup to understand the issue and propose a well-posed problem statement and a numerical solution strategy.

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A Posteriori Error Control and Adaptivity for the Finite Cell Method

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Key Words: finite cell method, a posteriori error control, adaptivity

The finite cell method is an immersed boundary method which combines a fictitious domain method with a (higher-order) finite element method [1]. Its basic idea is to replace the possibly complicated physical domain by an embedding domain of a geometrically simple shape which can easily be meshed. The variational formulation of the problem and its finite element discretization is defined on the embedding domain. The geometry of the physical domain is incorporated via an indicator function, which necessitates the implementation of an appropriate quadrature scheme.

The talk presents concepts of a posteriori error control for the finite cell method. The focus is on a residual-based error control for the reliable estimation of the discretization error with respect to the energy norm [2] and on the application of the dual weighted residual approach (DWR), which enables the control of the error in terms of a user-defined quantity of interest [3, 4]. In particular, the use of the DWR approach allows for the separation of the discretization error and the quadrature error. Both concepts of error control can be used to steer adaptive schemes for local mesh refinements. In several numerical experiments the performance of the error controls and the adaptive schemes is demonstrated.

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Efficient domain integration of discontinuous material using moment fitting method enhanced by neural network

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Key Words: *Moment fitting, Neural network, Weak discontinuity, Enrichment strategy*

As it removes the computationally expensive operation of generating the body-fitted mesh, the enrichment technique has been widely employed to consider structural discontinuities within an element. The standard shape function is locally hybridized with an enrichment function, enabling either state variable (e.g., displacement) or its derivative fields to contain discontinuity within the function. Irregularities such as jump, kinks, and other non-smoothness of a displacement field or its gradients are approximated, and the accuracy of the solution increases accordingly. The remarkable success of the techniques is based on the robustness and generality of the method, which is underpinned by the fact that the enriched function retains partition of unity properties. However, the enrichment techniques typically introduce a challenge in domain integration since the Gauss quadrature, which assumes Gauss-Legendre polynomial as an integrand, cannot be used in the standard form. Such changes, furthermore, often incur a high computational cost that is in proportion to the number of enriched elements, which is tied to the accuracy of the solution. For instance, in the extended finite element method (XFEM) [1], one of the most widely used enrichment methods, the number of Gauss quadrature points increases rapidly in proportion to the number of enriched elements.

This work introduces a novel method that calculates quadrature weights that adaptively change depending on discontinuity geometry. Inspired by a novel adaptive quadrature method presented recently [2], which reduces the computational load by fixing the number of integration points regardless of the discontinuity, we also combine the moment fitting method and the selective enrichment strategy. Additionally, we present a way to further accelerate computing the weights by leveraging the potential of the artificial neural network, a standard machine learning technique. Thanks to the nonlinear regression provided by the trained network [3], the computational overhead is minimized without sacrificing the accuracy of the solution: time-consuming operations- the calculation of the moments and the model's training-are done in the offline stage. Furthermore, we improve the solution accuracy without increasing the finite element grid by adjusting the moments by a detailed representation of the enrichment. We demonstrate the accuracy and efficiency of the proposed method by solving several numerical examples.

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Efficient Patient Specific Model Adaptation for in silico Bone Remodelling Prediction

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Key Words: Bone Remodelling, Image-Based Finite Element Analysis, Biological Factors

The development of tailor-made medical applications, such as personalised prosthetic implants benefits from the accurate prediction of short and long term bone remodelling simulation. The present work describes a numerical technique to reduce modelling errors through the derivation of patient-specific biological factors and physiological actions affecting this processes.

In the literature, the simulation of bone remodelling usually involves coarse estimations in the imposed physiological structural boundary conditions and the biological parameters included in the formulation of the remodelling algorithms. These generic assumptions, which introduce a large amount of modelling errors, are applied since the actual measurement of the modelling environment in each patient is not readily available in a practical medical protocol. In the proposed an optimization algorithm searches for the values of the sought patient-specific parameters. The optimization algorithm is driven by the error minimization between the obtained bone architecture after one remodelling cycle and a reference one, the CT scan image of the patient, assuming an homeostasis condition in the medical image. The bone remodelling algorithm used was proposed by Doblaré and García [1], while the tissue mechanical stimulus is computed using a immersed boundary methodology, the Cartesian grid Finite Element Method, since it is well suited for the generation of FE models directly from medical images [2].

A case study involving a pre-implantation human mandible CT scan image, suggests that the procedure is able to efficiently generate simulation conditions which are closer to those physiological observed in the medical image.

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Enrichment of Finite cells for Image-based analysis of Materials with complex Microstructures

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Key Words: Heterogeneous materials, computer tomography, least-squares fit, local enrichment, finite cell method

Numerical methods are widely used for solving engineering problems. For complex geometries, the finite cell method (FCM) - a combination of high-order finite elements with fictitious domain methods - is a promising approach [1]. Due to it's simple Cartesian grid, it is very efficient for modeling complex geometries. For smooth problems, the convergence rate is even exponential and therefore, the FCM performs very well. However, when dealing with heterogeneous microstructures coming from computer tomography (CT) scanner, such as, for example, hybrid metal foams or cemented sand, we face two challenges.

The first challenge is the non-smooth (staircase) geometry description given by the CT-scans. To increase the accuracy of the FCM, the geometry of the problem has to be smoothed. Here, a smooth geometry reconstruction based on a (cell-wise) least-squares fit is employed, which will be directly applied on the grayscale values of the voxel models, obtained from the CT-scans. This leads to a smooth levelset function, which then describes the geometry. This procedure has also the advantage, that it is directly applied on the raw data of the CT-scans, i.e. a time-consuming segmentation process will be avoided.

The second challenge is related to the heterogeneous materials, where the problem is not smooth anymore and thus, solving it becomes more challenging. Because of the different materials, weak discontinuities will occur at the material interfaces. These discontinuities are kinks in the solution, i.e. displacements, and jumps in the derivatives, i.e. stresses and strains. Since the FCM uses only smooth polynomials, it is not possible to capture the discontinuous part of the solution accurately and therefore, the convergence rate deteriorates. To overcome this issue, the FCM is extended by the local enrichment, which is based on the hp-d method combined with a high-order partition of unity (PUM) approach [2]. With this approach, the discontinuities in the heterogeneous materials can be captured very precisely.

In this contribution, the proposed approaches are explained and then, numerical examples are presented.

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Extended Spectral Cell Method For Explicit Dynamic Analysis in Structural Health Monitoring Applications

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Key Words: Spectral Cell Method, Enrichment, Mass Lumping, Explicit Dynamics, Guided Wave based Condition Assessment

In recent years, Guided-Waves (GW) based assessment has evolved into a potent field of Structural Health Monitoring (SHM). In this context, data driven methods are often found lacking. To boost performance, model-based evaluations can be used; these rely on transient analysis of simulations of the structure, where damage is detected by incrementally updating a numerical model as to match the recorded signal. In this task, the main challenge lies in providing an adequate Ansatz space for the simulation of high frequency modes, whilst automatically discretizing potentially complex structures and damage configurations. With the spectral cell method, voids in the domain can be represented independently from the mesh, while the Gauss-Lobatto-Legendre nodal configuration delivers high order shape functions, and enables the direct application of explicit solvers by virtue of the nodal quadrature method. This last advantage, however, is contingent on the use of mass lumping procedures over intersected elements, due to the customized quadrature rules used to resolve discontinuous integrands. For this, HRZ lumping can be applied as in Ref. [1], while an alternative based on moment fitting was recently suggested by the authors [2].

In this contribution, we aim at representing a more generalized set of features, such as cracks or inclusions. This is achieved via partition of unity enrichment functions, and a new moment fitting approach to lump the mass of enriched elements, resulting in a block-diagonal mass matrix. To render the mass matrix fully diagonal, eigenvalue decomposition of the system of equations can then be performed. We assess the stability of the method by considering a unit-size enriched element. Finally, its capabilities are demonstrated on the illustrative 3D modeling example of a cracked plate.

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Finite Cell Method using Boolean Operations for Multi-Material Problems

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Key Words: Finite Cell Method, Multi-Material Problems, Local Enrichment, Boolean Operations, Octree-Decomposition, Discontinuous Integrands

The Finite Cell Method (FCM), combining an unfitted discretization via Cartesian meshes and higher order shape functions, is an accurate and efficient tool, especially when it comes to the simulation of highly complex geometries [1]. The discontinuous integrals over cut elements are often computed using an adaptive integration scheme based on an Octree-Decomposition (OTD), resulting in a set of disjoint sub-cells over which the integral is computed individually. While the popularity of this approach is justified due to its robustness and easy implementation, high accuracy requirements often lead to a serious computational overhead due to the large number of generated integration points.

In our contribution, the Boolean FCM (B-FCM) approach proposed by Abedian and Düster [2] for porous media is further extended. Thus, the aim of this contribution is twofold: (i) application of the B-FCM to multi-material problems and (ii) combination with the local enrichment technique to accurately capture the weak discontinuities in the displacement field over cut cells in elastic problems [3]. The proposed B-FCM approach is based on the standard space-partitioning via OTD for integration purposes, however, it relies on Boolean operations. These are realized by introducing unique *Boolean labels* for each sub-cell. This serves two goals: (i) steering the OTD, such that a set of overlapping sub-cells is obtained in which the integration points can be distributed much more efficiently and (ii) modifying the integrand by Boolean operations over the individual sub-cells, such that the overlapping nature of the sub-cells is taken into account. Thus, the integral value over the entire cut cell is not changed. Using the proposed B-FCM approach, a significant reduction in the number of integration points by 70-80% can be obtained, which leads to major time savings when dealing with multi-material problems both in 2D and 3D applications. Furthermore, it should be noted that despite the impressive decrease of the number of integration points, the accuracy of the numerical integration is not affected.

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Improving the Robustness of the Finite Cell Method for Finite Strain problems

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Key Words: Large deformations, remeshing, condition number, eigenvalues, finite cell method

The finite cell method (FCM) is a combination of an immersed boundary method and high-order shape functions [1]. Since the geometry of the underlying problem is embedded into a simpler domain, it can be discretized using a Cartesian grid. This makes it suitable for modeling complex geometries such as structures generated from additive manufacturing or metal foam-like structures.

The Simulation of structures, including large deformations and finite strains, poses multiple challenges. The severe distortion of the mesh may significantly affect the accuracy and robustness of the numerical method and restrict it to smaller deformations than required. This problem is particularly present in the FCM, where complex geometries are discretized with a non-conforming Cartesian grid introducing a fictitious material with very low stiffness. In order to improve the FCM's robustness, we propose a global remeshing strategy to allow the nonlinear computation to proceed even for very large deformations where the distortion of the cells becomes significant [2]. The main idea is to perform a computation up to a specific deformation state where the distortion of the cells becomes critical. Afterwards, a new mesh is introduced to be able to continue the analysis.

Also, fictitious domain methods such as the FCM suffer from ill-conditioning especially when broken cells possess a very small volume fraction of the physical domain. One way to improve the conditioning is to introduce a very soft material in the fictitious domain. However, this method can modify the solution significantly because of the large stiffness added to the system. To this end, we apply and adapt a more efficient stabilization technique proposed by Loehnert [3] to improve the condition number of the FCM without affecting the solution significantly. In this approach, only the modes causing high condition numbers are stabilized for each broken cell, based on the eigenvalues of the cell stiffness matrix. The performance of the proposed methods will be illustrated using different numerical examples.

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Isogeometric V-reps: Efficient and Robust Integration

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Key Words: Isogeometric Analysis, Immersed Methods, Numerical Integration

We present an efficient and robust integration method to deal with volume representations (Vreps) in isogeometric analysis. In contrast to boundary representations (B-reps), the building blocks of V-reps are B-spline or NURBS (Non-Uniform Rational B-Spline) trivariates that generally involve trimming. While the related theories have been established in our precedent works [1, 2], here we focus on the corresponding algorithms to generate quadrature meshes for trimmed trivariates, including: (1) decomposition of a trimmed element into a collection of cells where the standard Gauss quadrature rule can be applied, and (2) reparameterization of the involved trimming surface in each cell as a Bezier surface. In particular, we adopt the marching-cubes cases [3] as the base cases and develop a corresponding decomposition for each of them to minimize the number of the resulting cells. Such a cell can be a hexahedron, wedge, pyramid, or a tetrahedron. On the other hand, trimmed elements that do not fit into one of the base cases are reparameterized using a novel strategy based on the use of folded decompositions [4]. In the end, we present several 3D examples to show the robustness of the proposed method.

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Links between ghost penalty stabilisation and aggregation-based finite element techniques

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Key Words: *Unfitted, embedded, immersed, finite elements*

In this work, we analyse the links between ghost penalty stabilisation [1] and aggregation-based discrete extension operators [2] for the numerical approximation of elliptic partial differential equations on unfitted meshes. We explore the behavior of ghost penalty methods in the limit as the penalty parameter goes to infinity, which returns a strong version of these methods [3]. We observe that these methods suffer locking in that limit. On the contrary, aggregated finite element spaces are locking-free because they can be expressed as an extension operator from well-posed to ill-posed degrees of freedom. Next, we propose novel ghost penalty methods that penalise the distance between the solution and its aggregation-based discrete extension. These methods are locking-free and converge to aggregated finite element methods in the infinite penalty parameter limit. We include an exhaustive set of numerical experiments in which we compare weak (ghost penalty) and strong (aggregated finite elements) schemes in terms of error quantities, condition numbers and sensitivity with respect to penalty coefficients on different geometries, intersection locations and mesh topologies. We will also discuss novel discrete extension operators that are well-posed for high order methods. Instead of considering extrapolations of the interior basis, we propose modified modal bases that do not involve high order extrapolation.

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Mathematical Aspects of the Shifted Boundary Method

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Key Words: Unfitted finite element methods; embedded methods; weak boundary conditions; Taylor expansions; high-order methods; shifted boundary method; consistency and convergence analysis.

The Shifted Boundary Method (SBM), introduced in [1], is an approximate domain method, falling in the broader class of un unfitted/embedded/immersed methods. In the SBM, the location where boundary conditions are applied is *shifted* from the true boundary to an approximate (surrogate) boundary, and, at the same time, modified (*shifted*) boundary conditions are applied. Since its appearance, the method has proven to be both flexible and robust in a variety of different applications, ranging from fluid-dynamics to solid mechanics, from heat transfer to electrostatics (see, e.g., the references in [2, 3, 4]).

The comprehension of the mathematical foundations of the method has accompanied its practical application in real-life situations. The analysis of the mathematical properties of the SBM highlights – in particular – sufficient conditions on the geometry, the unfitted mesh and the shifted boundary operator that guarantee the well-posedness of the SBM discrete variational formulation. This is accomplished through the fulfillment of suitable *coercivity* or *inf-sup conditions*, which can be checked in practice as they depend in an explicit way upon known quantities.

We will report our results in two different – somehow opposite – situations, namely the case of domains with corners [2] in which the physical solution is expected to exhibit singularities, and the case of domains with very smooth boundary, where the expected smoothness of the solution naturally suggests the use of a high-order approximation of the boundary operator [4]. We will also discuss the treatment of non-Dirichlet boundary conditions [3], as well as some open problems remaining in the analysis.

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Numerical Characterization and Evaluation of Additive Manufactured Parts in Geometrical Multiscale Computational Models

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Key Words: Finite Cell Method, Additive Manufacturing, Numerical Homogenization

Additive manufacturing (AM) in construction is a rapidly growing research field due to the increased geometric freedom, process automation and design optimization that it offers. The individualized part design promotes the construction of structural elements with exceptional physical properties. However, the realization of such elements highly depends on understanding the geometrical multiscale nature of the structures. As resolving the locally varying properties of AM components in a construction scale analysis is impractical, conventional structural analysis tools are not readily equipped to handle AM parts. A proper dimensional reduction process that can effectively deal with the geometric complexities of AM components is needed to represent the parts on the construction scale analysis.

In this contribution we propose such dimensional reduction process and illustrate its effectiveness in combination with a construction scale structural analysis. The dimensional reduction process can be realized by the homogenization of thermal and mechanical properties of the parts. By virtue of being a fictitious domain method with high-order finite elements, the Finite Cell Method (FCM) [1] is well-equipped to handle the individualized part geometries. Two cases with practical relevance are considered: a concrete wall element with internal cellular structures and a space frame with individualized 3D printed node topologies. In the case of the wall element, the thermal transmittance is chosen to represent the homogenized thermal behavior. The numerical results are validated by physical experiments. The bending and axial stiffness are used to characterize the homogenized mechanical behavior of the nodes. The numerical studies utilize massively parallel machines to solve large equation systems with many millions of unknowns [2], demonstrating the scalability of the approach to handle larger parts and complex constructions.

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On numerical integration of cut finite elements and cells

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Key Words: Fictitious domain methods, cut cells, numerical integration, quadrature, adaptive integration, octree, moment fitting, nonlinear problems, finite strains

Fictitious domain methods are of increasing interest since they do not require the generation of body-conforming finite element meshes. Therefore, fictitious domain methods are suited for problems with complex geometries. The finite cell method (FCM) is a combination of the fictitious domain approach with high-order finite elements. Thanks to the use of Cartesian meshes, the pre-processing, i.e. mesh generation is significantly simplified. Due to the fact that the applied meshes do not conform to the geometry of the problem, special care has to be taken with respect to the numerical integration of the weak form, the local refinement of the approximation as well as the treatment of boundary conditions.

The presentation will focus on the numerical integration of cut finite elements and cells arising in fictitious domain methods. First, a short overview of existing quadrature schemes will be given. Then, the moment fitting approach will be discussed in more detail. We will present some recent advances related to the moment fitting increasing its efficiency and robustness with respect to the computation of nonlinear problems. Emphasis will be placed on the question of how non-negative weights influence the robustness of the finite cell method. The investigations to be presented will range from the integration of polynomials and arbitrary functions to the solution of problems of solid mechanics applying the finite cell method. To this end, we will consider linear elastostatic problems as well as nonlinear solid mechanics problems including hyperelasticity and elastoplasticity at finite strains.

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Open-source NURBS handling toolbox in MATLAB

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Key Words: *NURBS, Open-source, cgFEM*

The most common CAD software in engineering use Non-Uniform Rational B-Splines (NURBS) to define the geometry of the models. This form of representation has important advantages from a design point of view, but it is a major obstacle for most CAE software. Only the most advanced finite element codes such as NEFEM or IGA preserve the NURBS representation of the geometries, while most commercial codes use approximate models.

Within the research line of the Cartesian grid Finite Element Method (cgFEM), we are interested in the numerical resolution of wave propagation problems. This type of simulation requires a faithful representation of the domain since small variations in the geometric model can lead to completely different solutions. The definition of geometry has consequences at many different stages of the analysis process (mesh-geometry intersection, operator evaluation, boundary condition imposition...) and it is necessary to have a wide range of tools for handling geometric issues. Although geometric modelling using NURBS is standard, to the author's knowledge, there is no library that offers all the necessary functionalities for analysis purposes.

In this work, we present the NURBSLAB toolbox. This MATLAB library contains all the functions we have developed for handling NURBS in the cgFEM context, and it is available to the scientific community under GNU license. We evidence the enhanced functionalities of our implementation in comparison with other available alternatives. We also show its application within the cgFEM framework and the use of some special features to improve the robustness of the analysis process.

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Penalized Direct-Forcing method and power-law-based wall model for Immersed-Boundary numerical simulations of obstacles in turbulent flow

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Key Words: Immersed Boundary Method, Penalized Direct Forcing, Explicit power-law wall model

This work is in the context of the safety-system development for the new generations of nuclear power plants. We wish to model the turbulent flow inside an industrial passive-safety device, the in-vessel flow limiter, based on the fluidic-diode principle [1]. Our goal is to design and optimize its shape. This shape optimization would need a lot of computations, each one with a specific mesh relative to the evaluated shape, followed by a statistical treatment.

In order to avoid the time consuming phase of re-meshing, we use the Fictitious Domain approach. Using an in-house industrial software, we face the constraint to not being able to modify the physical-problem governing equations in the code. Taking into account this fact, we choose the Penalized Direct Forcing method, a merge of the Penalty and Direct-Forcing (DF) methods [2]. It consists in a penalized forcing term, written in a DF formulation, added to the governing equations for taking into account the immersed boundaries.

Considering industrial turbulent-flow problems computed by RANS approach and not-resolved boundary layers, we need an appropriate immersed wall treatment. An immersed power-law-based wall model is chosen because its ability to model the velocity profile inside the whole boundary layer [3]. This is important due to the non-uniform distribution of the forced-node distances to the immersed wall. Moreover, this wall model has the advantage to be explicit and to not rely on an iterative procedure for the friction velocity determination. Therefore, coming from our previous directional linear interpolation technique [2], we have implemented the power law approach into our PDF method.

Using a Finite-Element version of our PDF method, we validate this approach on analytical-test cases and present our results concerning the in-vessel flow limiter industrial-test case.

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ϕ-FEM: a fictitious domain approach achieving optimal convergence without non standard numerical integration

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Key Words: Fictitious domain, levelset, optimal accuracy

Geometrically unfitted methods, i.e. the numerical methods using the computational meshes that do not fit the boundary of the domain, and/or the internal interfaces, have been widely used in the computational mechanics for decades. Their classical variants (Immersed Boundary or Fictitious Domain methods) are easy to implement but can suffer from poor accuracy. More recent approaches, like XFEM and CutFEM enjoy the optimal accuracy at the price of a considerable sophistication wrt the implementation: they introduce the integrals on the actual boundary and on the parts of the mesh cells cut by the boundary (the cut cells) so that a non trivial numerical integration is required.

In this talk, we present an alternative unfitted method – ϕ-FEM, first introduced in [1, 2], then extended to less academic problems in [3]. As in CutFEM/XFEM, we suppose that Ω is embedded into a simple background mesh and we introduce the active computational mesh $\mathcal{T}_h$, getting rid of the cells lying entirely outside the physical domain. The general procedure is as follows: we extend the governing equations from Ω to Ω_h (the domain of $\mathcal{T}_h$) and write down a formal variational formulation on Ω_h without taking into account the boundary conditions on $\partial\Omega$; we then impose the boundary conditions on $\partial\Omega$ using an appropriate ansatz or additional variables, explicitly involving the level set ϕ which provides the link to the actual boundary; finally, we add an appropriate stabilization to guarantee coerciveness/stability on the discrete level. This approach allows us to achieve the *optimal accuracy* using the usual FE spaces and the usual numerical integration: all the integrals in ϕ-FEM can be computed by standard quadrature rules on entire mesh cells and on *entire facets*. FE of *any order* can be straightforwardly used. The geometry is naturally taken into account with the needed optimal accuracy: it suffices to approximate the levelset by piecewise polynomials of sufficiently high degree.

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Simulation of Density-driven Subsurface Flow with a Phreatic Surface: Comparison of Approaches

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Key Words: Subsurface Flow, Phreatic Surface, Numerical Simulation, Level-Set Method, Finite-Volume Discretization, Ghost-Fluid Method

Numerical simulation of the density-driven flow in partially saturated aquifers is a challenging field of great practical importance. Robustness of the numerical methods should allow computations on domains whose geometry and hydrogeological structure approximate real-world geological formations (cf. e.g. [1]). The mobile liquid phase (solution of salt in water with variable concentration) saturates only a part of the domain. The flow of this phase is essentially influenced by dynamics of the interface between the saturated and unsaturated subdomains (the s.c. phreatic surface), as well as by gradient of the density.

In our talk, we consider two approaches for modeling this setting: The Richards-like model imposes a uniform system of PDEs in the whole domain [2]. In contrast to it, the phreatic surface can be considered as a moving boundary of the saturated subdomain and represented by the level-set approach. On this interface, the boundary conditions for the flow model are treated by the ghost-fluid method [3]. We compare these the approaches to investigate their limitations and computational aspects.

In our implementation, the systems of the PDEs are discretized by a vertex-centered finite-volume scheme. For the solution of the discretized systems linearized in the Newton's method, we apply the geometric multigrid method with ILU smoothing. The solvers is parallelized. We present results of the numerical experiments.

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Unfitted Finite Element Method for Fully Coupled Poroelasticity with Stabilization

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Key Words: *Condition number, Ghost penalty, Immersed boundary method, Nitsche's method, Poroelasticity, Unfitted finite element method*

The complex geometries of practical problems bring about a great challenge to the preprocessing of the standard finite element method (FEM), wherein the mesh conforms to the physical domain. An unfitted FEM with the physical domain embedded in a relatively simple mesh is a promising substitute for the fitted FEM for such cases. However, the use of the unfitted FEM for poroelasticity problems with continuous interpolation is seldom reported. Hence, in this paper, we propose a symmetric weak formulation based on the modification of Nitsche's method for fully coupled two-field poroelasticity. Furthermore, three stabilization terms based on the ghost penalty method are introduced to address the ill-conditioning caused by the extreme cut. The fluid pressure Laplacian method was employed to stabilize the pressure at the early stages in cases of small permeability and/or time step when P1P1 interpolations are employed.

The overall performance of the proposed methodology was evaluated through detailed numerical experiments. The methodology demonstrated excellent accuracy. The introduction of three ghost penalty terms enormously reduced the condition number, and the resulting condition number is at the same level as or close level to that of the fitted FEM. More importantly, they do not lead to great consistency errors, and the optimal convergence rates are preserved. Both the conditioning numbers and accuracies are approximately independent of the cut ratio. Furthermore, neither the accuracy nor the conditioning is very sensitive to the ghost penalty parameters.

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Voxel-based Simulations of Ductile Crack Propagation through Metal Matrix Composite Microstructures based on Eigenerosion and Finite Cells

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Key Words: Ductile fracture, Finite strains, Eigenerosion, Finite Cell Method, Metal Matrix Composites

In many engineering processes, e.g., mechanized tunneling, the efficiency of drilling processes strongly depends on the wear of the tools applied on the machine. In case of tunnel boring machines, cutting disks as well as chisels are used as mining tools, which consist of a metallic body armored by metal matrix layers. Those underlie the wear mechanisms abrasion and surface spalling. The latter is governed by subcritical crack propagation on the microscale under cyclic loads. Hence, the microstructure morphology and the material properties of the constituents strongly influence the resistance against crack propagation and thus against surface spalling.
In this contribution, a framework for the simulation of ductile crack propagation through metal matrix composite microstructures is presented. Therein, the eigenerosion approach as presented in [1] and its implementation for small strains in [2] are extended to an algorithmic scheme for finite strains and ductile fracture. For the ductile constituents, the finite strain J_2-plasticity formulation in [3] is applied. In order to efficiently simulate microstructures based on voxel data, an algorithm combining the extended Eigenerosion approach with the Finite Cell Method as introduced in [4]. As major part thereof, the mesh is refined adaptively at the crack tip by transforming the subcells of those finite cells at least containing one eroded subcell into single finite elements. The occurring hanging nodes are managed following [5]. In our approach, a special cell arrangement is constructed which minimizes the number of cells on the one hand and on the other hand, maintains a suitable aspect ratio of the cells' edge lengths. This aspect ratio may be irrelevant just for the integration in the subcells, but as soon as the subcells are transformed to separate elements at the crack tips the regularity of the elements becomes important. By evaluating results of simulations at the microscale, is it is shown that failure of the material can be investigated based on the proposed numerical scheme.

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A droplet-phase approach to solve thin-film flows

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Keywords: *Droplet-phase, Thin-film flows, SPH, DEM, 2D Manifolds*

Thin-film flows, observed in varied applications, are commonly seen in automobiles moving through rain. The prediction of the behaviour of such films is an important aspect that needs consideration during the design of vehicles with regard to their effect on exterior sensors, changes in aerodynamic behaviour, seepage of water into parts of the vehicle, etc. The droplet-phase model is a novel method that models the development and evolution of thin-films in the form of droplets. It consists of moving droplets on a 2-D manifold and allows the use of computational resources more efficiently in comparison to fully 3-D Navier-Stokes solvers to capture the same behaviour[1]. In the droplet-phase approach, the 2-D manifold contains droplets. The film height at a given location, is a function of the location of droplets in its neighbourhood. The momentum equation takes into consideration various forces that act on the droplet (hydrostatic pressure, viscous forces, etc.), and solves for the velocity of the droplets. The derivatives are estimated using weighting kernels and their derivatives, as in SPH. The advection of droplets at the solved velocity results in the evolution of the height function. In this approach, therefore, the evolution of the height function is captured through the movement of droplets that are treated as discrete particles, as in DEM, although the approach considered in the present work does not feature a contact model for droplet collisions. This facilitates the use of this approach for both DEM simulations such as droplets in free-flight as well as for thin-film flows. In this work, comparisons of the droplet-phase approach with shallow-water models are made for both 1-D and 2-D test cases. The results show the reliability of the method and highlight the potential of this method to solve problems with thin-films.

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A Lagrangian Meshfree Solution Scheme for Additive Manufacturing of Metals at Powder Scale

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Key Words: *meshfree methods, HOTM, thermomechanical coupling, additive manufacturing*

Powder-based Additive Manufacturing (AM) technologies, such as Powder Bed Fusion (PBF) and Directed Energy Deposition (DED) technologies, enable high degrees of design freedom for optimal functional features and customized products at reasonable costs. One of the leading research efforts in AM technology focuses on the rigorous product quality control by reducing the material defects in the microstructure and enhancing the reliability and robustness of the manufacturing processes. An attractive method for addressing this challenge is numerical modelling and predictive simulations [1-3]. We present a Lagrangian meshfree simulation scheme for AM technologies of metals at the powder scale based on the Hot Optimal Transportation Meshfree (HOTM) method [4]. In the simulations, metallic powder particles are modelled explicitly as deformable bodies according to their size and shape distributions measured in experiments. The strongly coupled thermomechanical response of the material is simulated by a thermo-viscoplasticity model. The conservation of linear momentum and energy equations are solved simultaneously to predict the deformation, temperature and phase evolution of the particles. The computational framework is capable of predicting the granularity and fine-scale physics in the problem, such as powder particle thermodynamics, material phase evolution and fluid-structure interactions, which primarily affect the mechanical behaviour and heat transfer in the aggregation of discrete particles [5]. Furthermore, high-fidelity predictions of the defect formation in the microstructure of 3D printed metallic parts, including voids, micro-cracks, unmelted/partially melted second phase inclusions, can be achieved. The proposed approach is validated in the applications of Laser PBF-AM process and DED technologies of metals.

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A novel implicit material point method for ductile fractures

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Key Words: MPM, phase field, ductile fracture

Predictive modelling of ductile fracture is of extreme interest to the engineering community as it pertains to various applications, e.g., fracture propagation in metal alloys. Cracks propagating in solids are governed by complex phenomena such as crack initiation, multiple crack branching, or crack arrest. Mesh distortion errors that are inevitable in large displacement FEA hinder the fidelity of such simulations where the deformability of mesh affects the resulting contact forces and corresponding failure surfaces.

Material point methods have been shown to provide high fidelity solutions for domains undergoing large displacements and/or large strains [1]. Rather than relying on the notion of a deforming mesh, material point methods introduce a particle based approximation for the deformable body that move within a non-deforming mesh. This introduces a considerable advantage as opposed to purely particle based methods as the continuum approximation is preserved thus releasing the requirement for high particle densities.

To this point, material point implementations for brittle fracture have proven efficient in tackling quasi-static crack propagation in terms of computational simplicity and robustness. The Phase Field Material Point Method (PF-MPM) has been successfully introduced [2] for quasi-static brittle fracture problems. In this, the phase field is resolved at material points and mapped onto grid nodes where the phase field governing equations are solved.

In this work, the PF-MPM is originally extended to account for fractures propagating in ductile materials. A NURBS based background grid is deployed to treat cell-crossing errors. Driven by the developments in [3] the basis is properly extended at the boundaries to provide stable fracture patterns. The merits of the proposed scheme are investigated through a set of benchmark cases.

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Discrete Element Simulation of Compaction and Sintering of Ceramic Powders

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Key Words: *Powder Compaction, Sintering, Ceramic, Discrete Element Method*

The Finite Element Method (FEM) is an established method for the simulation of powder metallurgy processes on a large scale. However, it cannot explicitly consider the particulate nature and the composite aspect of powders. An alternative simulation method is the Discrete Element Method (DEM) which considers each particle and its interactions with its neighbors. For large-scale problems, these are challenging simulations due to the high computational cost associated with representing a very large number of particles.

In the present work, we present a DEM model that can simulate two important stages of the powder metallurgy process: compaction and sintering. We use the in-house developed code dp3D [1] dedicated to materials science. Spherical discrete elements in the code model porous agglomerates which indent each other during compaction and sintering.

In the compaction process, uniaxial die compaction, using an upper and lower punch, has been implemented on a cylindrical geometry. The process kinematics are decomposed into a compression stage, unloading, and ejection of the pellet. Interactions between the particles and the die are considered elastoplastic, by implementing and adapting a large-density model [2]. A qualitative approach is followed in the sintering process, using the Bouvard Pan model [3, 4].

The results are in good agreement with experimental data and FEM simulations, regarding stress-strain curve, density gradient, elastic spring-back, and final geometry. The simulations show that the friction coefficient is the primary factor to induce a density gradient in the pellet. The pellet is more porous in its center when compared to the regions close to the punches. This density gradient induces a non-homogeneous sintering, which results in a final geometry that is no longer cylindrical. This so-called diabolo effect in the sintered pellet was previously simulated by FEM, but to the author's best knowledge, it is the first time that it has been reproduced by DEM.

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Force method conception using transfer matrix to apply to multiphase flow by one-by-one corresponding Particle-Cartesian cell (*P*/*CC*) model

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Key Words: *Force method to continuum mechanics, Transfer matrix method, Multiphase flow, Cauchy-Riemann equations, Conjugate variables, One-by-one corresponding Particle-Cartesian cell model, Locking-free finite element method*

The objective of this study is to develop a force method for application in the multiphase flow by the one-by-one corresponding Particle-Cartesian cell model, which is previously proposed in [1].
Displacements and forces continue at the surfaces between phases, whereas strains discontinue. Meanwhile, the proposed force method is applicable for continuum mechanics and differs from the conventional method for the framework, and it is referred to as Continua-work in this study. In this study, two types of schemes are presented: the first is as follows, and second is built using the so-called separation parameter method.

The state vector: {displacement, stresses}: $\{\boldsymbol{U},\nabla\boldsymbol{F}\}$ continues and the strains represented by $\{\nabla\boldsymbol{U}\}$ discontinue in general to satisfy the week solution of the virtual work according to the FEM conception. One of the proposed force methods uses incomplete three-fold third-order element, consisting of parameter vector: $\{\boldsymbol{U},\nabla\boldsymbol{F}\}_k$ on the vertex node k. Therefore, the element function is represented by parameter vector: $\{\boldsymbol{U},\nabla\boldsymbol{F},\nabla\nabla\boldsymbol{F},\cdots\}_0$ on the local origin. The strains are represented by $\{\nabla\boldsymbol{F}/\nu\}$ of the transfer matrix, where ν is kinetic viscosity.

The transfer matrix, also known as the reduction matrix, can represent state vector $\{\boldsymbol{U},\nabla\boldsymbol{F}\}_b$ on b by state vector $\{\boldsymbol{U},\nabla\boldsymbol{F}\}_a$ on a, even though a rigid member (rigidity $G = \infty$) is included. This is because the forces are transferred, and they continue at the boundary. In beam theory, it exists as a strong solution; however, for continua, it exists only week solutions.

The simultaneous equation is constructed by the virtual work principle. Cauchy-Riemann equations defined in two dimensions must be satisfied as necessary conditions for a robust scheme because the strain and stress represented by $\{\nabla\boldsymbol{U},\nabla\boldsymbol{F}\}$ have four components (freedom). In the same way in three dimensions, as constraint conditions, so-called conjugate variables concept has been proposed.

Accordingly, the equilibrium equation represented by $\{\boldsymbol{U}\}_k$ and $\{\nabla\boldsymbol{F}\}_k$ for multiphase flow represented with different ν has been obtained. In addition, another scheme is explained in the full paper.

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Modeling of Solid Phase Processing of Aluminum Alloys using Smoothed Particle Hydrodynamics and Physics-Based Constitutive Material Model

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Abstract

Solid Phase Processing (SPP) is a high-strain process applied to materials during fabrication to produce high-performance alloys, semi-finished products, and engineered assemblies without the requirement to melt the constitutive materials. This emerging manufacturing platform delivers extraordinary performance in metal alloys, relative to identical materials produced by conventional manufacturing routes. Friction Stir Welding/Processing (FSW/FSP), Friction Stir Extrusion (FSE), and Shear Assisted Processing and Extrusion (ShAPE) are some of the advanced manufacturing techniques part of the SPP family. Simulation of such processes remains an ongoing challenge in computational mechanics and computational material science. There are difficulties associated not only with the formulation of physics-based models to accurately predict material behavior at the solid-state, but also with the computational methods required to treat extremely large material deformation. A physics-based material model accounting for the attributes from lower length-scale, such as grain size, dislocation density, dynamic recrystallization and recovery, to the bulk thermomechanical material behavior with varying strain rate and temperature history will be presented. This model was incorporated into a continuum-scale smoothed particle hydrodynamics (SPH) model to simulate FSP, FSE, and ShAPE tube extrusion of aluminum alloys. Due to its inherent meshfree and Lagrangian feature, SPH model is well-suited to modeling processes with severe deformation. Numerical results are validated with the experimental data, demonstrating a promising structure-properties linkage achieved by the model. The proposed physics based SPH model leads to an improved prediction and better understanding of the microstructural evolution and thermomechanical behavior of the material across SPP processes, enabling an accelerated and cost-effective development effort.

Modelling of forming processes using the Particle Finite Element Method (PFEM).

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Key Words: *Forming processes, thermo-mechanical problems, Particle methods, PFEM*

In this work we present the latest advances in the Particles Finite Element Method (PFEM) for the numerical modeling of forming processes. In the recent past, very good results of the method have been shown in the simulation of 3D cutting problems. The method has very good capabilities for treating large deformations in massive volumetric parts. Now the method is applied and extended to other forming operations: forging, blanking, minting, machining, etc., for metals and other materials.

One of the important aspects of these manufacturing techniques is the interaction with the molds and dies. Deformable contact interactions are needed to obtain a close correspondence between numerical and experimental results. The characterization of the thermomechanical interaction with the coatings of the tool plays an important role. Advances have been made in meshing techniques for treating three-dimensional parts and for the modeling deformable contact.

The characterization of friction and wear of the forming tools can be modeled considering also the lubrication on the surfaces. The purpose is to obtain the characteristics of the final shape of the workpiece, the areas that experience large plastic deformations and the residual stresses that remain in the processed material. This information is very valuable for the optimal design of the manufacturing operation.

To show the virtues of the method, several examples of forming operations are presented. The capabilities of the method are discussed, as well as the accuracy of the solutions.

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Multiscale, multiphysics modeling of wave propagation in anisotropic saturated porous media

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Key Words: *Multiscale modelling, hydro-mechanical coupling, wave propagation, saturated soil, anisotropy*

We present an innovative multiscale, multiphysics coupling approach to solve a class of dynamic problems in saturated granular media. The approach is formulated by coupling dual-phase material point method (MPM) with the discrete element method (DEM), where the MPM is used to solve macroscopic deformation and pore pressure of saturated porous media while the DEM is attached to each material point to derive the nonlinear mechanical response of the solid matrix of porous media. Based on the Terzaghi's effective stress principle, the DEM receives deformation gradient from its attached material point to compute the effective stress quantities for the MPM and the pore fluid is considered by the continuum method MPM via the *u-v-p* formulation. A semi-implicit integration scheme is derived to circumvent the limitation on small-time steps imposed by incompressibility of interstitial fluid and the potential low permeability. The developed approach is further employed to model the wave propagation in saturated anisotropic granular sand. We demonstrate that multiscale simulation can capture a rich array of patterns of wave propagation and offer direct link and explanation of these phenomena with their underlying microstructural mechanisms.

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Particle-based Numerical Analysis of Jet Flow from a Pipe

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Key Words: *Particle-based Flow Analysis, Jet Flow, Boiling Heat Transfer*

Cooling processes are widely used in steel making processes. In some processes, plates are cooled using water flowed from pipes. Generally, cooling is performed in which water is dropped onto a steel plate by its own weight from a plurality of pipes.

In the cooling process, there is a heat transfer coefficient as an index showing the cooling capacity. In the case of steel making process, boiling heat transfer is dominant. The heat transfer coefficient at boiling condition can be estimated by the surface temperature of the plate, the water density, and the collision pressure.

However, a large amount of cooling water from a plurality of pipes stays on the plate as water pool. It is difficult to estimate the pressure that collides with the actual plate because it is cooled from above the water on the plate. Therefore, the collision pressure during cooling of the jet flow above the water pool was analyzed by the particle-based flow analysis, which is excellent in free surface analysis.

The accuracy of the calculation was confirmed by comparing with the experimental results. As a result, the experiment and the calculation showed that the larger the amount of water in the pipe laminar the higher the collision pressure tended to be. Flow analysis using the particle method has made it possible to estimate the heat transfer coefficient under a complex free surface where water pool and jet flow interfere.

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Passive self-propulsion based on asymmetric collision dynamics.

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Key Words: DEM, bi-elastic, self-propulsion, symmetry breaking, asymmetric collisions, energy harvesting

It has been a long discussion on the possibility to convert random Brownian motion to usefull work, also known as thermal energy harvesting, for over a hundred years in various gedankenexperiments [1]. The concept based on the Brownian ratchet deemed impossible [2]. Recently, an attempt to check the concept of Brownian ratchet using macroscopic granular gas was undertaken, showing principial possibility to convert random motion to usefull work [3]. Granular gas may perform work directly as Smoluchowski ratchet, and even more effieiently, if bi-sided (elastic and inelastic) vains are used. The question still remains, whether it is possible to build a microscopic system, converting thermal motion to work ? An asymmetric sawtooth potential might do that yielding directed current, if the particles are periodically heated and cooled [4]. We approach the problem of converting random motion to the directed one from the other side. Instead of making asymmetric external conditions, like a ratchet or a potential, we make particles asymmetric. If sides of a particle have a different restitution ratio, then it yields asymmetric collision dynamics, thus favouring certain post-collision direction. We show the main idea based on a simple collision model and present the results of DEM simulations of bi-elastic particles' ensemble.

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SPH simulation of landslides as a multi-physics problem

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Key Words: SPH, Landslides, Multi-physics Problems, Finite strain elastoplasticity

Landslides are among the most dangerous geologic hazards there are. One example of a catastrophic event was observed in 2016, when an earthquake magnitude M7.3 triggered a series of landslide disasters in Kumamoto prefecture, Japan. Such event had serious consequences, one of the most remarkable being the collapse of a 200 m long bridge called Aso bridge. Given its large-scale nature, it is of great importance to develop numerical methods to study it. However, it is still to be seen a numerical method capable of accurately predict and evaluate the post-failure behavior of a landslide in an unified simulation. In this context, we propose a Smoothed Particle Hydrodynamics (SPH)-based multi-physics approach to simulate the complete landslide phenomena.

For the stable solid part of the landslide, we propose a total Lagrangian SPH formulation for Solid Mechanics problems [1] with finite strain elastoplastic stress update that can be easily adapted to any plastic yield criteria. Then, ruptured particles according to a simple rupture criterion such as establishing a threshold on the accumulative plastic strain are assigned to change its physical status to become a non-Newtonian fluid. The ruptured particles are considered to be the flowing part of the landslide, which we solve with a fully implicit Incompressible SPH (IISPH) method [2]. Finalizing the method, we arrange the coupling mechanism as a fluid-structure interaction problem in a similar way as [1]. In addition, we developed a solid-solid contact algorithm for SPH that include both the non-penetration condition and friction forces to enable the inclusion of debris material into the landslide flow.

Numerical tests include simple verification and validation examples such as the triaxial compression test with the modified Cam–Clay constitutive model. Finally, we show the robustness of the proposed method with a simulation of the Aso landslide taking the earthquake loading into account.

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The P-DNS Method to Solve Particle-Laden Turbulent Fluid Flows

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Key Words: *Multiscale Solutions, Turbulent Flows, Particle-Laden Fluids, P-DNS*

Particle-laden flows refer to a kind of two-phase fluid flow in which one of the phases is continuously connected and the other phase is made up of small immiscible particles. Two-phase flow modeling has a wide variety of scientific and engineering applications: dispersion of contamination in the atmosphere, fluidization in combustion processes, deposition of aerosols in aerosol drugs, spread of virus in the air, rain formation in clouds, sand and dust storms, protoplanetary disks, volcanic eruptions, geological sedimentation processes, pharmaceutical sprays, liquid-fueled combustion and solid rocket motors, are examples of engineering processes that involve particle-laden flows among many others.

The equations governing interactions of particles with fluids in a particle-laden mixture have been known for many decades. However, their coupled dynamics often result in complex behavior such as preferential concentration and turbulence modulation. These are still ongoing topics of research. The starting point for a mathematical description of almost any type of fluid flow is the classical set of Navier–Stokes equations (N-S). To describe particle-laden flows, these equations must be modified for the effect of the particles.

Typically, the fluid is treated in a Eulerian frame, while the particles are treated in a Lagrangian way. However, problem with the Lagrangian treatment of the particles is that once the number becomes large, it may require a prohibitive amount of computational power to track a sufficiently large sample of particles required for statistical convergence. In addition, if the particles are sufficiently light, they behave essentially like a second fluid. This is the main objective of this presentation.

On the other hand, due to the interactions between turbulence structure and dispersed particles, turbulence characteristics of momentum and heat transport can be modified by the presence of particles. This last phenomenon is known as turbulence modulation and can lead to a significant increase or decrease in the parameters that regulate turbulence.

The authors presented in Ref. [1] a multi-scale method called Pseudo-Direct Numerical Simulation (P-DNS) [2] to study the phenomenon of turbulence modulation in a particle-laden flows. However, in that article, the particles in both, the fine scale and the coarse scale, were treated in a discrete way moving in a Lagrangian reference frame within the fluid. In this presentation, the same P-DNS method will be used to simulate the presence of particles as a continuum function that moves within the fluid. The result is similar to a fluid mixing problem, with the exception that now the coefficients that regulate the convection of one fluid with respect to the other, are obtained from a direct numerical simulation obtained on a finer scale solved offline. In this way, the need to represent each of the particles that move in the fluid is avoided.

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Towards a Quasicontinuum Method for Granular Systems

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Key Words: Discrete Element Method, Quasicontinuum Method, Granular Materials

The Quasicontinuum (QC) Method [1] was developed for quasi-static atomistic simulations where the arrangement of atoms is calculated to minimise the global potential energy of the system by using a reduced number of atoms. The method thereby reduces the number of degrees of freedom of the problem which in turn reduces the computational cost of the simulation. In pursuit of a QC method for granular systems, an implicit integration scheme for the Discrete Element Method (DEM) [2], based on the variational integrator approach [3] is developed [4]. This combines an integration scheme that is compatible with the variational structure of the QC method with a fully dynamical description required for granular systems.

This talk will extend our previous work by introducing the coarsening technique of the QC method to the dynamics of granular systems. In accordance with the QC method, a series of representative particles (or rep-particles) are chosen which become the degrees of freedom of the coarsened system and particle momenta, mass and forces of regular particles are mapped to rep-particles. The density of rep-particles can be low in regions where particles tend to experience little relative motion (such as the low inertial regime) and gradually increased in regions where higher deformations are expected. Rep-particles can be reallocated while the simulation runs and the gradual transition in rep-particle density avoids the need for handshake or boundary regions.

An overview of the QC method will be presented along with comparisons to classical DEM simulations. Our implementation of the QC method shows good statistical agreement with DEM simulations.

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An Isogeometric Analysis Based Topology Optimization Framework for Additive Manufacturing of 2D Cross-Flow Heat Exchangers

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Key Words: *Topology Optimization, Cross-Flow Heat Exchanger, Isogeometric Analysis, Heat Exchange Performance, Pressure Drop, Manufacturing Constraints*

Heat exchangers (HXs) have gained increasing attention due to the intensive demand of performance improving and energy saving for various equipment and machines. As a natural application, topology optimization has been involved in the structural design of HXs aiming at improving heat exchange performance (HXP) and meanwhile controlling pressure drop (PD). In this paper, a novel multiphysics based topology optimization framework is developed to maximize the HXP between two fluids with different temperatures for 2D cross-flow HXs, and concurrently minimize the PD between the fluid inlet and outlet. In particular, an isogeometric analysis (IGA) solver is developed to solve the coupled steady-state Navier-Stokes and heat convection-diffusion equations. Non-body-fitted control mesh is adopted instead of dynamically remeshing the design domain during the evolution of the two-fluid boundary interface. The method of moving morphable voids (MMVs) is employed to represent and track boundary interface between these two different fluids. In addition, various constraints are incorporated to guarantee proper manufacturability of the optimized structures with respect to practical manufacturing process such as additive manufacturing. To implement the iterative optimization process, the method of moving asymptotes (MMA) is employed. Numerical examples show that the HXP of the optimized structure is greatly improved compared with its corresponding initial design, and the PD between the fluid inlet and outlet is minimized concurrently. Moreover, smooth boundary interface between two fluids and improved manufacturability are also obtained for the optimized structures.

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An Open-Source Immersogeometric Analysis Framework for Heart Valve Modeling and Simulation

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Key Words: *Immersogeometric Analysis, Heart Valves, Isogeometric Analysis, Fluid-Structure Interaction, Open-Source Software, FEniCS*

Prosthetic heart valves have been simulated for nearly a decade [1,2], but all state-of-the-art research codes have remained in-house. This work outlines an open-source framework that is capable of industrial-scale, physiologically accurate heart valve simulations. This framework utilizes the open-source finite element software FEniCS [3] and its isogeometric extension, tIGAr [4]. The novel contributions to the simulation framework, building on the work of Kamensky et al. [5], include adding an arbitrary Lagrangian–Eulerian reference frame to the fluid problem, implementing the solid problem for the artery walls, and the inclusion of accurate material models for the artery walls and valve leaflets. These contributions enable prosthetic heart valve simulations that perform comparably to other cutting-edge analysis programs. Additionally, because of FEniCS's large user community, our framework is easier to learn, pre-process simulation inputs, and post-process results when compared to in-house codes.

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Isogeometric Analysis for Automotive Body Structure using Splines with Extraordinary Points

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Key Words: *Isogeometric analysis, Splines with extraordinary points, Trimmed NURBS, Crash Simulation, 3-point bending*

In order to improve CAE accuracy and reduce the manpower needed to transition from CAD to CAE, the use of isogeometric analysis (IGA) is an efficient approach for automotive applications. To make crash simulation models based on IGA, we started using the outer and inner trimming functions. For the parts of the body in white, approximately 80% of all parts were made using the outer trimming function. Outer trimming function is very effective and fast to generate IGA models. However, it was not a suitable option for very complex parts and parts having big holes like outer panel around the doors. Therefore, for the remaining approximately 20% of all parts, inner trimming function was initially adopted. By using this function, outer panel model was completed. However, this inner trimming function resulted in some issues. The presence of some small elements in the model was hard to avoid, which limited the size of the time step. In addition, time-consuming reconstruction work for CAD surfaces was needed. More importantly, border lines between NURBS surfaces were weakly C^0-continuous. Thus, once fracture occurs, the fracture tends to progress along the C^0 boundary which suggests that the fracture patterns are affected by the discretization of the geometry. To resolve these issues of trimmed NURBS, we used splines with extraordinary points to represent the outer panel [1, 2]. By using splines with extraordinary points, the model for the outer panel was made very fast, there were no small elements in the model limiting the time-step size, and the geometry was at least C^1-continuous everywhere. The axial crush, 3-point bending test, and simulations with hat section frame were performed to investigate the accuracy of splines with extraordinary points. It was found that splines with extraordinary points are more effective for obtaining results with high accuracy.

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Isogeometric analysis in LS-DYNA: advances in industrial deployment

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Key Words: Isogeometric analysis (IGA), (un)structured splines, trimming, crashworthiness, LS-DYNA

In this communication we review recent developments in isogeometric analysis in LS-DYNA. We outline currently supported geometric representations, reveal novel analysis features, and demonstrate their use through selected examples. We discuss the role and importance of hybrid models comprised of Lagrange polynomial as well as spline-based discretizations as industrial deployment of the technology progresses towards production grade.

Isogeometric Reconstruction and Crash Analysis of a 1996 Body-in-White Dodge Neon

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Key Words: *Crash, isogeometric analysis, CAD, Ricci flow, quadrilateral layout*

Isogeometric analysis (IGA) has attracted attention from academia and industry because of its high-fidelity results, ability to represent geometry exactly, and potential to streamline the engineering design-through-analysis process. However, one of the greatest challenges limiting the scope of IGA is the ability to rapidly convert CAD geometry into a set of splines suitable for engineering analysis—particularly for a wide set of shapes of industrial relevance.

In this presentation, we describe a new, mathematically rigorous, potentially automatable framework using Ricci flow and subsequent metric optimization [1] through which surface geometries can be rebuilt as sets of watertight, analysis-suitable, boundary-conforming semi-structured NURBS patches. Reconstruction of models using this framework leads to geometries that are immediately suitable for both isogeometric analysis and any additional design operations.

We demonstrate the utility of this method by rebuilding a trimmed CAD model of the US Army's DEVCOM Generic Hull vehicle [2] as a set of watertight splines. We also reconstruct the chassis of a 1996 Dodge Neon [3] from a finite element model as a set of analysis-suitable splines.

Finally, we perform crash analysis of the Dodge Neon vehicle using the reconstructed spline spaces. It is shown that the Bezier elements of the isogeometric splines can be much coarser than the quadrilateral and triangular elements of the original finite element model while still producing analysis results with much higher accuracy than those of the original model. (Here, accuracy is determined by comparing analysis results with those on refined finite element meshes.) Ultimately, this work both showcases a high-fidelity isogeometric model reconstruction paradigm and also affirms the merit of isogeometric analysis in automotive crash simulations.

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Isogeometric shell analysis for aerospace engineering applications

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Key Words: Isogeometric Analysis, Aerospace Engineering, Aircraft Structures, Penalty Coupling

While isogeometric shell analysis has many significant advantages in the design and simulation of complex science and engineering problems involving thin structures, several key challenges remain in establishing isogeometric analysis (IGA) as a robust and reliable industry standard for computational analysis. This work focuses on developing adaptable modeling and analysis approaches that enable the direct and effective use of IGA for aerospace engineering applications. The capabilities of these developments are demonstrated through the modeling, simulation, and analysis of aircraft structures.

For airframes that include numerous curved geometries that conform to the airfoil surfaces of the aircraft, IGA provides a suitable alternative to traditional finite element approaches because of its capabilities in modeling exact geometries. However, the complex designs of the airframe structures in an aircraft's wings, stabilizers, and fuselage require methods to connect multiple geometric components in the aircraft model. This is accomplished through a patch coupling method that applies to many different geometric configurations and problems through the use of dimensionally consistent penalty terms [1]. This coupling approach enables efficient analysis of the aircraft's internal support structures. Material modeling approaches are developed to identify different material property regions and subdivide the airframe structures for consistent analysis. In the future, the effective application of these approaches could also facilitate developing direct inputs to improve the design of various aircraft components within an analysis-driven computational design framework.

The presented simulation and modeling approaches for these aircraft applications highlight the adaptability and design power of incorporating IGA as an analysis tool in the aerospace industry. These developments support further improvements in computational analysis-driven design approaches for a variety of complex structures, including for aircraft applications, and offer an important step toward optimizing the efficiency, performance, and cost of many types of structures.

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An Interpolating Particle Method for the Vlasov–Poisson equation

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Key Words: particle method, Lagrangian scheme, Vlasov–Poisson equation, reproducing kernel Hilbert spaces

The Vlasov–Poisson equation is high-dimensional and develops strong turbulences. Therefore grid-based methods rapidly become expensive and thus infeasible to use. Particle methods try to overcome these problems by avoiding a phase-space grid and instead moving weighted particles along their respective trajectories. While computationally less expensive, traditional particle methods produce noisy results with low convergence rates and therefore need high resolutions and remapping strategies.
We present a particle method which avoids this noise by interpolating the correct function values at each particle-position without resorting to a grid in phase-space. Furthermore using RKHS-theory we can show that interpolation using an appropriate kernel leads to optimal convergence rates.

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Interpolating Vortex Particle Methods using Spline Wavelets

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Key Words: vortex methods, particle methods, interpolation, splines, wavelets

Vortex particle methods are Lagrangian schemes for the vorticity formulation of the incompressible Navier–Stokes equations. Because they make use of stream functions and are based on the analytical solution of the advection equation, they possess many favourable properties: a complete absence of numerical visocity, exactly divergence-free velocity fields, no CFL condition, no LBB condition, and many more.

In this talk we extend our previous work [1] on splines for particle methods. This approach allowed us to perform long-term accurate, high-order simulations without remeshing and could compete with a state-of-the-art discontinuous Galerkin method. However, when flows develop steep gradients and particles begin to cluster the method becomes inefficient due to its lack of adaptivity.

We then present a novel approach that instead interprets a given particle cloud as a set of point values and constructs smooth interpolants on them. These interpolants make use of spline wavelets and are adaptive. On the one hand, the method is a natural extension of our previous approach. On the other hand, there is a close relationship with radial basis function interpolants. The resulting schemes have many beneficial properties and preliminary results are promising.

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PROPERTY-PRESERVING DISCONTINUOUS GALERKIN METHODS FOR HYPERBOLIC PROBLEMS

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Key Words: Algebraic flux correction, discontinuous Galerkin methods, hyperbolic problems, limiters

Discontinuous Galerkin (DG) methods are among the most widely used numerical discretization techniques for solving partial differential equations. Their local conservation property, high order accuracy, and favorable scalability in parallel make these schemes attractive for many applications in computational fluid dynamics.

There are however, many shock-dominated problems, for which DG methods fail to produce approximations free of spurious oscillations, and might even crash. To overcome this shortcoming, we blend a provably property-preserving low order method with the corresponding high order DG target scheme. The proposed method extends the recently developed monolithic convex limiting procedures, designed originally for continuous finite elements [3, 4] to the DG setting. This algebraic flux limiter is primarily used to impose local (and global) bounds on numerical approximations [2] but extensions for incorporating entropy inequalities, as well as relaxation of the constraints in smooth regions are also possible.

In my talk, I will discuss the details of the approach, which include the sparsification of the low order method, stabilization of the numerical flux, as well as the design of the monolithic limiter. Sequential limiting for products of unknowns (originally proposed in [1]) and the preservation of global constraints, such as nonnegativity of pressure will also be touched upon. The performance of the method is evaluated for a variety of classical benchmarks for scalar conservation laws, as well as the systems of shallow water and Euler equations.

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Recent Advances in Pressure-robust Finite Element methods

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Key Words: Navier–Stokes Equations, Pressure-robustness, Finite Element Methods

The talk focuses on a certain family of pressure-robust finite element methods based on the idea by Alexander Linke to modify the test functions, see e.g. [1]. Pressure-robustness is a favorable property of a numerical scheme if large irrotational forces appear in the momentum balance, e.g. through external forces, the material derivative or coupling terms. In case of incompressibility the irrotational parts of the forces should be fully balanced by the pressure. The velocity of a discrete scheme that is not pressure-robust may show large errors if this pressure is relatively complicated and there even can be observed a locking phenomenon with respect to the viscosity in the simplest incompressible Stokes setting.

The talk shortly recalls the ideas with some well-known finite elements and demonstrates in particular how the Bernardi–Raugel finite element method can be modified into a pressure-robust scheme of lowest order with the same number of degrees of freedom that heals the shortcomings mentioned above. Similar ideas can be used to design a well-balanced scheme for the compressible Navier–Stokes equations that also preserves mass and non-negativity of the density [2].

It is not straight-forward to preserve pressure-robustness (even for fully divergence-free schemes) in convection stabilization and (guaranteed) a posteriori error control. The talk also presents some latest progress on these issues that are mainly based on studying the underlying vorticity equation [3, 4].

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A robust and accurate SPH formulation for compressible multi-phase flows

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Key Words: *SPH, Multiphase Flows, Meshless Methods, CFD*

Multiphase flows are frequently encountered fluid phenomena in a large range of cutting edge science and engineering problems, e.g. underwater explosion and cavitating flows. In terms of the numerical modeling of compressible multi-phase flows, the mesh-based methods are normally employed. Although SPH, as a meshless method, is inherently suited for the modeling of sharp interface problems, which has already been proven successful in industrial incompressible flows [1], the application in modelling strongly compressible multi-phase flows is still rare, mainly due to its inability to maintain a stable and accurate solution at the phase interface.

In this work, we present a robust and accurate SPH formulation for the numerical modeling of multi-phase flows with strong compressibility. An adaptive and extended Riemann solver is developed to handle materials with general equations of state and large density ratio. Numerical dissipation is applied adaptively considering the local smoothness of the flow field. The scale of SPH particles is evolved dynamically according to the local flow features to increase the efficiency of simulation. A second-order gradient estimator as well as the MUSCL-Hancock scheme are utilized to go beyond 1st order of accuracy. The proposed method is implemented in the code developed in [2]. Extensive numerical tests are carried out to validate the accuracy of the proposed numerical method in the end. Significant improvement is observed comparing to traditional SPH. The simulation results exhibit low dissipation while are able to maintain a smoothed pressure field in the mean time.

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Molecular Dynamics Simulation on Dynamic Behaviors of Nanodroplets Impinging on Wrinkle Surfaces of Graphene

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Key Words: *Nanodroplet, Molecular dynamics simulation, Impinge, Graphene*

The phenomenon of droplets' impinging on a solid surface is common in engineering applications. With the application of micro and nanotechnology in industrial processes, the impinging behavior of nanodroplets has aroused widespread interest. Graphene can be easily induced ripples and wrinkles in most cases due to its thermodynamic instability. In this paper, a series of wrinkled graphene models of sinusoidal morphologies are established, and molecular dynamics simulation is used to explore the dynamic process of nanodroplet impinging on the solid surface. The effects of nanodroplets with different droplet velocities, wrinkled graphene models of sinusoidal morphologies with various parameters, and different solid surface energy on the dynamic characteristics of nanodroplets are discussed and analyzed.

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SPH Modeling of Cavitation Impact on Soft Tissue Material

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Key Words: *Finite Viscoelasticity, TLSPH, Cavitation*

Collapsing gas or vapor bubbles may induce violent liquid jets that can create pores in membranes or tissue. These pores can be fundamental for transport processes of medicine or genes to target cells. Therefore, further investigation of the underlying physical mechanisms can improve the biomedical treatment of drug delivery and other medical applications.

We apply the meshless smoothed particle hydrodynamics (SPH) method to simulate cavitation and bubble collapse processes near soft tissue. Using the total Lagrangian SPH (TLSPH) formulation enables us to simulate viscoelastic tissue-mimicking materials. TLSPH is an extension of the conventional SPH method, which is often proposed for simulation of tensile instability processes and, hence, for simulation of solid materials undergoing large deformations. We obtain the properties of the soft tissue materials from the basic hereditary integral formulation and the generalized Maxwell model for finite-strain viscoelasticity theory, allowing for a combination of viscoelasticity and hyper-elasticity. Given the complexity of soft tissue material properties, an efficient continuum damage model is considered to evaluate the damage degree of particles, together with the SPH method to capture the resulting discontinuous damage. This combination of methodologies allows for modelling of damage and failure behaviour of soft tissue surrounded by a liquid.

This SPH solver will be tested for several cases of bubble collapses attached to or detached from the soft tissue. Compared to other coupling approaches using different methods, the selected SPH approach is able to capture fluid and solid responses straightforward and simultaneously, naturally satisfying the momentum conservation and saving computational resources.

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A conjugate gradient solver based on adapted deflation for the efficient solution of large scale, 3D crack propagation problems using eXtended/generalised finite elements.

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Key Words: XFEM, GFEM, deflated CG, multigrid, domain decomposition

The eXtended/Generalised Finite Element Method (XFEM/GFEM) has significantly contributed towards the increase of the level of automation and computational efficiency of crack propagation simulations. The method substantially reduces, or even eliminates, the need for re-meshing by employing Partition of Unity (PU) enrichment, which extends the Finite Element (FE) approximation space to include functions encompassing known features of the solution. In fracture mechanics, features such as discontinuities and singularities can be represented independently of the underlying mesh, offering significant computational advantages. However, for large scale three-dimensional problems, the most computationally demanding part of the process is the solution of the resulting linear system of equations, which is typically performed using iterative solvers, such as the Preconditioned Conjugate Gradient (PCG) method. The XFEM/GFEM is known to produce ill-conditioned matrices, which can significantly slow down convergence of such methods, while discontinuities can also negatively affect the performance of commonly used preconditioners, rendering the overall solution process inefficient.

In the present work, a preconditioner based on adapted deflation [1] is employed to accelerate the solution of linear systems resulting from the discretization of fracture mechanics problems with well-conditioned extended/generalized FEs [2]. A novel approach is proposed for the construction of the deflation space, where the space typically used for linear elasticity problems is enriched with additional vectors, accounting for the enrichment functions used, thus effectively removing low frequency components of the error. To further improve performance, deflation is combined, in a multiplicative way, with a block-Jacobi preconditioner, which removes high frequency components of the error as well as linear dependencies introduced by enrichment. The resulting scheme is tested on a series of non-planar crack propagation problems and compared to alternative linear solvers in terms of performance.

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A Discontinuity-enriched Finite Element Method for Dynamic Brittle Fracture

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Key Words: Discontinuity-enriched Finite Element Method, Dynamic Fracture, Linear Elastic Fracture Mechanics, Discrete Time Integration, Crack Propagation

The finite element method (FEM) is the standard procedure for modeling dynamic fracture but requires finite element (FE) meshes fitting to cracks. The eXtended/Generalized finite element method (X/GFEM) [4] elegantly decouples the description of cracks from the FE discretization by enriching or enhancing the standard FEM space. Yet, X/GFEM suffers from issues that are inherent to the formulation, including lack of stability, the need for non-standard procedures for prescribing non-zero Dirichlet boundary conditions, and an intricate computer implementation.

As an alternative to X/GFEM, the Discontinuity-enriched Finite Element Method (DE-FEM) [1, 6, 3] was proposed recently to solve problems with both material interfaces and cracks with a unified formulation. By collocating enriched nodes directly along discontinuities, DE-FEM also decouples cracks from the background FE mesh while solving X/GFEM's aforementioned issues. Yet, DE-FEM has only been explored so far for stationary cracks under stationary loading. In this presentation we demonstrate DE-FEM to simulate dynamic brittle fracture. We study the method in combination with both Newmark's constant average acceleration method and Bathe's method [2], and we use a fracture propagation criterion based on stress intensity factors obtained by means of a dynamic interaction integral [5]. Results show DE-FEM is an alternative to X/GFEM for solving dynamic brittle fracture problems.

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A Scale-Bridging Generalized Finite Element Methods for Structural Dynamics and Wave Propagation

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Key Words: GFEM; XFEM; Multiscale; Structural dynamics; Wave propagation; Global–local analysis

This presentation reports on a high-order multiscale Generalized Finite Element Method (GFEM) tailored for the solution of structural dynamics and wave propagation problems exhibiting fine-scale and/or localized solution features such as singularities and discontinuities [1]. The proposed method uses an explicit time-marching scheme together with a block-diagonal lumped mass matrix applicable to arbitrary patch approximation spaces and adopts shape functions computed numerically on the fly through the solution of local initial/boundary value problems. Numerical results in for problems exhibiting singularities in the spatial gradient show that the proposed GFEM can accurately capture relevant features of the response using structural-scale meshes that are much coarser than those required by Direct Generalized Finite Element Analyses (DGFEAs) of comparable accuracy. In addition, a detailed study of the critical time step size of the method is presented and compared against the one for DGFEA discretizations that provide similar levels of accuracy. It shows that the proposed method has considerably looser time step size restrictions than available DGFEAs.

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Model-based Simulations of Laser Lithotripsy Using a CutFEM Method

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Key Words: CutFEM, Laser Ablation, Nitsche's Method

In this work, a model of thermal ablation with application to multi-pulsed laser lithotripsy is presented. The approach is based on the one-sided Stefan-Signorini model for thermal ablation and the CutFEM discretization, described in Claus et al.[1]. The model relies on a level-set function to represent the moving interface between the solid phase and a fictitious gas phase (representing the ablated material). Consistent with a CutFEM approach, the interface geometry is allowed to be arbitrary with respect to a background finite-element mesh. Nitsche's method is adopted to impose the Signorini condition on the moving interface. A bound constraint is also imposed to deal with the thermal shocks that can arise during representative simulations of pulsed ablation with high-powered lasers. We report simulation results based on experiments for pulsed laser ablation of BegoStone samples in dry conditions. The model is calibrated against experimental measurements by adjusting the percentage of incoming laser energy absorbed at the surface of the stone sample. Model-based simulation results are validated against experimental observations for the crater depth, volume, and geometry as a function of laser pulse energy and duration. Our results illustrate how the spreading of the laser beam from the fiber tip is necessary to model in order to obtain a qualitative match with the experiments. In particular, the model-based simulations indicate that ablation saturates after a finite set of pulses.

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Space-Time Enriched Finite Element Methods for Wave Propagation

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Key Words: Generalized Finite Elements; Space-Time Methods; Plane-Wave Enrichment; Wave Equation; Elastodynamics.

Generalized finite elements based on plane-wave enrichments have been shown since the late 1990s to significantly reduce the computational cost for the numerical approximation of wave propagation and scattering problems in the frequency domain [2]. The enrichment of the approximation space allows good approximation of highly oscillatory solutions even on coarse mesh grids whereas standard methods are limited by fine meshes and small time steps. Recently enriched methods have been extended to time-dependent problems, using time-independent enrichment functions [2, 4, 5]. They reduce the computational effort in space, provided tiny time steps are chosen. In this talk we discuss space-time enriched methods for transient wave propagation on coarse space-time meshes [3]. We present a finite element method based on discontinuous Galerkin approximation in time and continuous elements in space, with plane-wave enrichments in space and time. Numerical experiments compare this approach to standard (polynomial-based) Trefftz methods [1] and to enriched methods based on time-independent enrichments [2]. For model problems in two-dimensions we demonstrate the significant reductions in the required computational effort and the rapid convergence of the proposed method on a fixed space-time mesh. We also discuss the influence of high condition numbers on the numerical solution, as well as the straight-forward extension to elastodynamics.

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Time-dependent modelling of quasi-brittle materials with a strong discontinuity approach

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Key Words: Time-dependent behaviour, Discrete Crack Approach, Finite Element Method, Coupled Algorithm

The time-dependent behaviour of quasi-brittle materials can have a significant effect on serviceability and ultimate failure. E.g., in the case of concrete structures, the presence of cracking can evolve, propagate and gradually widen over time, therefore significantly changing the stress state and expected structural response. The development of models that can account for the discrete nature of cracking whilst predicting time-dependent behaviour can be of interest to many practical applications. The discrete strong discontinuity approach (DSDA) has been validated as a reliable formulation for simulating the cracking phenomenon by directly embedding the traction-separation constitutive relation within finite elements, therefore enabling (or enriching) standard finite element models with the ability to capture cracks, where material can separate without the need for remeshing. This work presents a generalisation of the DSDA to account for the long-term behaviour of cracked quasi-brittle materials, more specifically creep and shrinkage. To this end, a rate-type creep is first applied through a number of kelvin units; the interactive behaviour of the resulting response from the Kelvin chain system, shrinkage, and discrete cracking is developed to obtain a suitable constitutive model for the discrete crack simulations. Finally, the formulation is deployed on a finite element code where the performance of the proposed model is assessed through representative numerical examples.

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XFEM based electrostatic analysis for edge effect of parallel plates

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Key Words: Extended finite element method, Electrostatic field analysis, Laplace problem, Conformal mapping, Complex function, Newton-Raphson iteration

In this presentation, we propose an extended finite element method that can effectively analyze the edge effect of the parallel plates capacitor.

The enrichment function, which plays an important role in this method, is defined as a simple function in the virtual space using the conformal mapping. The gradient of the enrichment function is also defined in the virtual space using the complex velocity potential. The enrichment function and its gradient are mapped into the real space by inverse mapping and used for numerical integration.

It is also very difficult to perform this inverse mapping analytically. We have performed it numerically, using the domain decomposition into triangles and the Newton-Raphson iterative scheme for complex numbers.

The effectiveness of the proposed method is verified by numerical experiments. To quantitatively evaluate the accuracy, we use the L_2 error norm of the solution and its gradient. The proposed method shows smaller error norms than the classical finite element method for equivalent resolution meshes.

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A Consistent Multiphase Flow Model with Incompressible SPH for 3D Bubble Rising Problems

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Key Words: Multiphase flows, Smoothed particle hydrodynamics, Inompressible SPH, GPU computing, Particle shifting

A multiphase flow solution method developed with the incompressible smoothed particle hydrodynamics (SPH) method is outlined in this contribution. We will present a generalized particle shifting method for multiphase flows that maintains particle regularity, prevents interface particle mixture, and only introduces minimal perturbation to momentum conservation and system energy. The aforementioned generalized particle shifting method has been improved from the original method proposed in [1], and has demonstrated better solution accuracy and higher efficiency compared to the original method and the optimized particle shifting method [2], respectively. A color-function-based repulsive force will also be introduced in the presentation, which regulates the magnitude of repulsive force by the color function and effectively improves the interface smoothness especially for multiphase flows with high density ratios.

This solution approach employs consistent discretizations for the gradient and Laplacian operators, which enhances the accuracy of the spatial differential operators. The surface tension model embraced relies on the continuum surface stress (CSS) formulation. The solution methodology proposed is broadly applicable and the solution robustness can be preserved with density ratios up to 1:1000, and viscosity ratios up to 1:100. Numerical results for a series of benchmark problems will be presented to demonstrate the accuracy of the proposed model by comparing simulation results against analytical solutions, results from other numerical methods, and experimental data. The simulation of 3D bubble rising problems raises challenges on computational efficiency [3]. The proposed model has been implemented on GPU, which enables its capability to solve complex physics phenomena encountered in 3D bubble rising and coalescence problems via simulations that include over one million SPH particles.

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An accurate and stable high-order particle method for droplet dynamics with interface coalescence and breakup in 3D

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Key Words: *Particle method, high-order schemes, stability, droplet, free surface, surface tension*

The droplet flow in the air can be simplified to a free-surface flow when the gas velocity is not high. The Lagrangian particle method is suitable for such flows. Nevertheless, the accurate and stable implementation of surface tension at free surfaces is still challenging. Recently, Matsunaga *et al*. [1] demonstrated that surface tension can be considered as a boundary condition at free surfaces based on a moving surface mesh. However, the surface mesh made it complicated and difficult to extend the method to 3D and simulate topological changes of interfaces. The aim of this study is to develop an accurate and stable particle method in 3D for droplet dynamics via replacing the surface mesh by the detected free-surface particles.

The surface tension is considered as a Dirichlet pressure boundary condition at free surfaces [1]. To enhance accuracy, the ***high-order schemes*** in our previous study [2] are employed instead of the ***conventional conservative schemes***. When the free surface particles are directly used, there are two well-known challenging problems: (a) the *instability* due to the mistaken free-surface detection [1, 2] and (b) the *fluctuation* of the detected free-surface boundary. To solve the first problem, the mechanism how the mistaken free-surface detection triggers fast error growth (i.e., instability) is analyzed theoretically and numerically. It is found that the summation of the discretization-model coefficients is closely related with the instability. Thus, *novel indices based on the discretization-model coefficients* are proposed for free-surface detection to suppress the instability. For the second problem, a new *surface-normal particle shifting* (SNPS) technique is proposed to alleviate the fluctuation of the detected free-surface boundary. Specifically, a smooth free-surface boundary is reconstructed based on the curve fitting method. Then the free-surface particles are gradually shifted to the reconstructed boundary. Based on these techniques, the stability of high-order schemes can be greatly enhanced for droplet dynamics with free surfaces.

Various numerical examples verified/validated the methods and demonstrated the improvements. The hydrostatic pressure and dam break problems demonstrated that the proposed indices detected fewer free-surface particles but produced better stability. The droplet deformation, coalescence, and breakup cases in 3D verified the method and demonstrated that the SNPS could greatly reduce the fluctuations and improve the accuracy. Briefly, it is well known that ***the high-order schemes*** suffer from ***instability*** easily ***at free surfaces***. The ***proposed techniques*** can effectively ***suppress the instability problem***.

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An ML-Accelerated Polygon Solid Boundary Technique for MPS Method

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Key Words: *Polygon Boundary, Ghost Particles, Machine Learning (ML), Moving Particle Semi-implicit (MPS)*

Solid boundaries are omnipresent in fluid simulations. Their accurate treatment remains an open and challenging topic for particle-based methods such as the Moving-Particle Semi-implicit (MPS). The main issue stems from the incompleteness of the kernel function near solid boundaries. The most common technique to handle this deficiency is using a set of ghost or fictitious particles, which help compensate for the kernel truncation. These particles can be pre-determined or dynamically positioned during simulation. They also help in producing the boundary forces and assigning boundary conditions. Nevertheless, even for two-dimensional models, this process can quickly become a bottleneck for particle methods when the wall geometry is complex (e.g., terrain) or moving.

The present study proposes a novel technique enabled by a Machine Learning (ML) approach that properly treats solid boundaries in fluid numerical simulation. Conventional ghost boundary particles are replaced with a fictitious polygon that encapsulates the behavior of all ghost particles. To achieve this with the help of an ML technique, a training data set for various boundary shapes are generated from simulations using the dynamic ghost particle method. The features of the rendered ghost particles are recorded, such as formation, solid-fluid interface, trimmed effective area, particles resolution, and particle number density. Symbolic states are specified and tagged manually. The label on each class describes how to mitigate kernel incompleteness according to its category. The saved data then serves to train a multiclass classification model. Once the ML model is trained, it estimates required boundary impact parameters (e.g., particle number density) on polygon represented boundaries (without ghost particles). The simulation results demonstrate the effectiveness of the new ML-accelerated technique in increasing the computational efficiency while maintaining the accuracy as equal to the standard ghost particle method, especially near sharp boundary edges.

Least Squares Based Particle Method for Accurate Free-surface Flow Simulation

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Key Words: *Computational Fluid Dynamics, Incompressible Flow, Surface Tension, Meshfree Particle Method, Polynomial Reconstruction*

Meshfree particle methods, such as the SPH and MPS methods, have been attracting a great deal of attention, particularly in the engineering field, due to their high versatility for complicated physical problems including free-surface flow. However, the accuracy of these conventional particle methods is in general much lower than that of the prevalent grid-based methods. On the other hand, the least squares moving particle semi-implicit (LSMPS) method proposed by Tami and Koshizuka [1] is featured by an arbitrary high order accuracy. Nevertheless, the LSMPS method tends to be numerically unstable in the presence of large free-surface deformations. For these reasons, an accurate simulation of free-surface flow has been remained as a great challenge for meshfree particle methods.

Aiming at accurately and stably simulating a free-surface flow, we have developed two novel particle methods based on least squares. One of them is the moving surface mesh particle method [1], in which a moving surface mesh is incorporated to improve the treatment of free-surface boundary. The 2nd-order LSMPS scheme is adopted as the spatial discretization scheme. The numerical stability is effectively improved because of the use of the moving surface mesh. Highly accurate solutions have been obtained for surface tension dominant flows, such as droplet oscillation, dripping faucet, and continuous inkjet. However, the application of this method is limited to problems without complex topological changes such as the generation of splashes.

Another new particle method we have developed is a stabilized LSMPS method which is aimed at the accurate simulation of complex free-surface flow. In order to improve the numerical stability in the vicinity of the free surface, calculation algorithms for handling free surfaces and splashes are overall modified, where the surface fitting technique is incorporated to accurately and robustly estimate the normal vector to the free surface. Furthermore, the LSMPS scheme is extended by incorporating additional techniques (namely, Tikhonov regularization, diffuse derivative constraint, and linear equality constraint) to stabilize the spatial discretization. The proposed method has been applied to several benchmark problems, and consequently, the high accuracy is demonstrated for problems with free-surface deformations of moderate to high complexity.

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MPS for modeling of multiphase granular flows: capabilities and limitation

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Key Words: Multiphase granular flow, Particle methods, Continuum-based modeling, MPS method, Multi-resolution model

Continuum-based particle methods, such as moving particle semi-implicit (MPS), provide the opportunity to simulate the multiphase granular flows with more accuracy and flexibility than the Eulerian mesh-based methods, and better computational efficiency than the discrete-based particle methods. Here we investigate the capabilities and limitations of these continuum-based particle methods for the gravity-driven and fluid-driven multiphase granular flows with different regimes (i.e. quasi-static, dense flow, and kinetic regimes). The model of this study is based on a multi-resolution, weakly-compressible moving particle semi-implicit (WC-MPS) with various stability and accuracy enhancement techniques. It used a generalized rheological model, using a regularized visco-inertial rheology that can describe the granular behavior in all regimes of multiphase granular flow. The result of the model is evaluated for the gravity-driven case of immersed granular collapse/slide, and the fluid-driven case of dam-break over an erodible bed, in comparison to the experimental data and discrete element method (DEM) results.

The results demonstrate the ability of the models in dealing with the large deformations in granular flows. A high sensitivity of results to the tensile instability (in high-shear regions) and unphysical fluctuations is observed. The enhancement techniques prove to be effective in improving the failure and post-failure behaviors of granular materials. The grain to particle size ratio is found to be a crucial factor in the accuracy of granular simulations. The multi-resolution technique shows to be effective and essential to keep the spatial resolution of the granular phase large enough for satisfying the continuum assumption, without scarifying the resolution and accuracy of the model for the fluid phase.

Surface Tension and Negative Pressure Calculation using Moving Particle Hydrodynamic Method

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Key Words: *Particle methods, Surface tension, Wettability, Negative pressure, MPS, SPH, MPH*

Particle methods can calculate free surface flows without explicit surface tracking, and surface tension is of importance in properly capturing the surface motion especially in small scale problems. However, the surface tension calculation in particle methods has intrinsic difficulty because the tension in particle methods often results in strange agglomeration, which is called tensile instability. This instability also emerges in negative pressure calculations. To overcome this difficulty, the potential force which is long-range attractive and short-range repulsive is applied in some surface tension models [1-3]. It is expected that such potential based surface tension models are also useful in calculating the negative pressure. In this study, the potential based surface tension model [3] are diverted for negative pressure calculations (Fig.1) and their performance is studied using moving particle hydrodynamics (MPH). The pressure is directly evaluated with the interaction force via the virial theorem standing on the physical consistency of the discrete formulation in the MPH method.

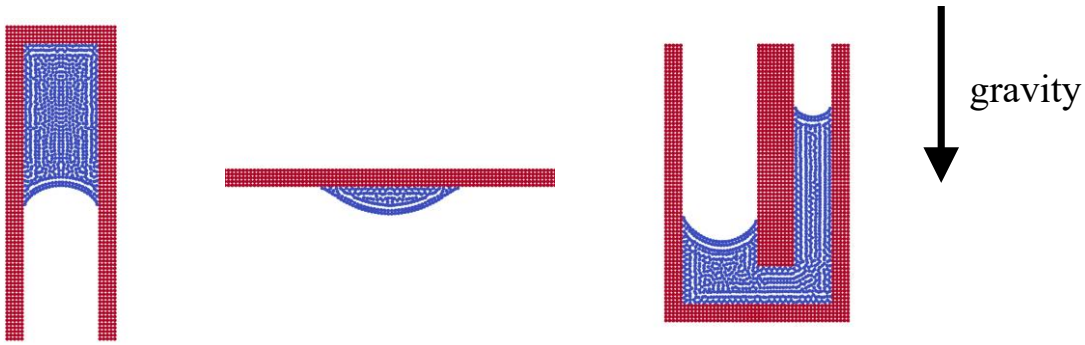

Fig. 1 Capillary calculations with negative pressure

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An adaptive framework for analysis-aware defeaturing

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Key Words: Defeaturing, trimming, geometric simplification, adaptivity

Defeaturing consists in simplifying geometrical models by removing the geometrical features that are not relevant for simulation. For instance, in solid mechanics simulations, they can be holes or fillets away from stress concentration regions. Simplifying the geometry of a computer aided design (CAD) model by defeaturing enables more efficient simulations for engineering analysis problems: the resulting mesh is simpler, the computation faster, and less memory storage is needed. However, the effects of defeaturing on the accuracy of the analysis are often neglected: it is a time-consuming task that is often performed manually and based on the expertise of engineers. Understanding well the effects of this process is an important step to be able to adaptively integrate design and analysis for CAD/CAE.

In this talk, we will formalize the process of defeaturing by understanding its effect on the solution of partial differential problems defined on the geometrical model of interest. More specifically, we have developed an *a posteriori* estimator of the energy error between the solutions of the exact and the defeatured geometries, that allows us to control the error made by adding or removing geometrical features. To this estimator, we have also integrated the numerical error due to the numerical approximation of the problem at hand when using hierarchical B-spline based isogeometric analysis on trimmed geometries.

The dependence of the estimator upon the size of the features and of the mesh elements is explicit, and the effectivity index is independent from the number of features considered. The estimator is proven to be reliable, it can be computed very efficiently, and it is naturally parallelizable with respect to the number of features. Finally, we propose a refinement strategy based on the estimator. It adaptively determines the mesh elements to refine, and chooses the features that are needed in the geometrical model, in order to achieve a certain precision.

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An Optimally Convergent Smooth Blended B-spline Construction for Unstructured Quadrilateral and Hexahedral Meshes

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Key Words: Isogeometric analysis, B-splines, smooth splines, quadrilateral meshes, hexahedral meshes.

Easy to construct and optimally convergent generalisations of B-splines to unstructured meshes are essential for the application of isogeometric analysis to domains with non-trivial topologies. Nonetheless, especially for hexahedral meshes, the construction of smooth and optimally convergent isogeometric analysis basis functions is still an open question. We introduce a simple partition of unity construction that yields smooth blended B-splines, referred to as SB-splines, on unstructured quadrilateral and hexahedral meshes [1]. To this end, we first define the mixed smoothness B-splines that are C^0 continuous in the unstructured regions of the mesh but have higher smoothness everywhere else. Subsequently, the SB-splines are obtained by smoothly blending the mixed smoothness B-splines with Bernstein bases of equal degree. One of the key novelties of our approach is that the required smooth weight functions are assembled from the available smooth B-splines on the unstructured mesh. The SB-splines are globally smooth, non-negative, have no breakpoints within the elements and reduce to conventional B-splines away from the unstructured regions of the mesh. Although we consider only quadratic mixed smoothness B-splines, the construction carries over to arbitrary degrees. We demonstrate the excellent performance and optimal convergence of SB-splines studying Poisson and biharmonic problems.

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Analysis-Suitable T-Splines of Arbitrary Dimension and Degree

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Key Words: Isogeometric Analysis, analysis-suitable T-splines, multivariate T-splines

T-splines were introduced in 2003 in computer-aided design as a new realization for B-splines on non-uniform meshes with local mesh refinement, and they were soon applied in the context of Isogeometric Analysis as ansatz functions for Galerkin schemes, however linear dependencies might occur in rare cases. In 2012, it was shown that linear independence is guaranteed if T-junction extensions do not intersect in different directions [1]. This criterion is called *analysis-suitability* and is equivalent to *dual-compatibility* [2], which states the existence of a dual basis that is constructable via local knot vectors. Analysis-suitability was generalized to bivariate T-splines of arbitrary polynomial degree [3], and, in an abstract version, to multivariate T-splines of odd degree [4].

In this contribution, we give a dimension-independent definition of analysis-suitable T-splines of arbitrary degree, including even and mixed degrees. We generalize both approaches to analysis-suitability, the abstract and the geometric one, and argue that both are sufficient for linear independence of the corresponding T-splines.

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C^1 Hierarchical Spaces on Multi-patch Domains for Isogeometric Methods

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Key Words: Multi-patch C^1 spline spaces, hierarchical splines, isogeometric analysis

In recent years there is a considerable development of locally refinable spline spaces, due to their application to create adaptive algorithms for modelling, approximation and analysis. In particular, in Isogeometric Analysis (IgA), it was proved that using hierarchical splines leads to efficient methods for the solution of PDEs with optimal convergence rates (see, e.g., [1] for an overview). Moreover, combining IgA with C^1 spline spaces defined on multi-patch domains is a natural way to handle high-order problems on complex geometries. Therefore, there is the need for such kind of spaces which at the same time allow local refinement. Our approach combines recent techniques for the construction of C^1 tensor-product spaces (see, e.g., [3, 4]) with a new hierarchical framework (having relaxed assumptions with respect to the standard one). In this way, and by employing the results available for the two-patch case [2], we are able to obtain the desired locally refinable C^1 continuous spline spaces defined on multi-patch geometries.

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Isogeometric Analysis based on Modified Loop Subdivision Surface with Optimal Convergence Rates

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Key Words: Loop subdivision, Isogeometric analysis, Optimal convergence rates, Nitsches technique

This paper introduces a modified version of Loop subdivision, called modified Loop subdivision surface (MLSS), to achieve optimal convergence rates in isogeometric analysis. Two main ideas are introduced to define MLSS. Motivated by the open knots for B-splines, we add a new layer of basis functions for the boundary of control grid, which can be evaluated similarly as that for Loop subdivision basis functions. This idea is used to solve the non-optimal convergence rates problem for extended Loop subdivision even without extraordinary points (EPs). For the EPs, we define a new rule with a parameter $\lambda(0 < \lambda < 1)$, which is exactly the second maximum eigenvalue of the subdivision matrix. The MLSS is defined by combining the two ideas, which is global C^2-continuous except G^1 and curvature bounded around the EPs. The MLSS limit surface has comparable shape quality as Loop subdivision surface. Besides that, the numerical experiments show that MLSS can achieve optimal convergence rates in the Poisson problem both in the L_2 and H_1 norm.

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Kirchhoff-Love Shell Representation and Analysis using Triangle Configuration B-splines

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Key Words: *Isogeometric analysis, Kirchhoff-Love shell, TCB-splines, extraordinary points*

This paper presents the application of TCB-splines for representing and analyzing the Kirchhoff-Love shell in the context of isogeometric analysis (IGA). The Kirchhoff-Love shell formulation requires globally C^1-continuous basis functions. The nonuniform rational B-spline (NURBS)-based IGA has been extensively used for developing Kirchhoff-Love shell elements. However, shells of complex geometries inevitably need multiple patches, where stitching patches with high continuity is a challenge. On the other hand, due to their unstructured nature, TCB-splines can accommodate general polygonal domains and are flexible to model complex geometries with C^1 continuity, which naturally fit in the Kirchhoff-Love shell formulation with complex geometries. We propose to use TCB-splines as basis functions for both geometric representation and solution approximation. We apply our method on shell benchmark problems, where optimal convergence rates are achieved. The applicability of the proposed approach to shell analysis is further exemplified by performing geometrically nonlinear Kirchhoff–Love shell simulations of an oil sump of a car and a pipe junction represented by a single patch of TCB-splines free of extraordinary points.

Stabilized Overlapping Multi-patch Isogeometric Formulation of the Stokes Problem

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Key Words: *Stabilized Method, Overlapping Patches, Trimming, Union, Stokes Problem, Isogeometric Analysis*

We present a novel stabilized isogeometric formulation for the Stokes problem, where the geometry of interest is obtained in the means of overlapping NURBS (non-uniform rational B-spline) patches, i.e., one patch on top of another in an arbitrary but predefined hierarchical order. All the *visible* regions constitute the computational domain, whereas independent patches are coupled through visible interfaces using Nitsche's formulation. Such a geometric representation necessarily involves trimming, which, however, may yield trimmed elements of extremely small measures (referred to as *bad elements*) and thus lead to the instability issue. Motivated by the *minimal stabilization* method that rigorously guarantees stability in problems using trimmed geometries [1, 2], in this work we generalize it to the Stokes problem on overlapping patches. Central to our method is the distinct treatment for pressure and velocity spaces, where stabilization for velocity is carried out for the flux terms on interfaces, whereas pressure is stabilized in all the bad elements. We provide a priori error estimates with a comprehensive theoretical study. Through a suite of numerical tests (particularly with two-dimensional Taylor-Hood elements), we first show that optimal convergence rates are achieved, which consistently agree with our theoretical findings. Second, we show that the accuracy of pressure is significantly improved up to several orders using the proposed stabilization method, compared to the results without using stabilization. Finally, we also demonstrate the efficacy and efficiency of the proposed method in an advection-dominated problem, i.e., the Oseen problem.

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A Radial Basis Function Partition of Unity Method for Thin Structures

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Key Words: Radial basis function, partition of unity, anisotropic, unfitted, least squares

Computational modelling of thin structures is a challenging problem. If variations in the thin direction can be neglected, shell elements can be used to simplify the problem and to reduce the computational cost. However, if this is not the case, also the thin direction needs to be resolved. A uniform discretization, e.g., through meshing, leeds to a high computational cost, since the extent of the structure along the surface is large compared with the thickness. A global anisotropic discretization is difficult to construct and to work with if the structure does not have a parametric representation.

Meshfree methods provide flexibility with respect to geometry, but have similar limitations with respect to discretization of thin structures. In [1] an unfitted least-squares radial basis function partition of unity method (RBF-PUM) was derived. The main benefits of unfitted least squares RBF-PUM are that it is stable under node refinement, that node generation becomes trivial, and that it is computationally efficient due to its local support and the reusability of local computations.

We have formulated an adapted version of unfitted least squares RBF-PUM that is suitable for thin structures. An RBF-PUM discretization is based on local approximations in overlapping patches that are then blended together to form a global solution. Typically patches are uniformly distributed and equally sized cubes or spheres, but we instead use anisotropic patches in the form of cylinders that are aligned with the structure, such that the heights of the cylinders are similar to the thickness of the structure. Within each patch we can then control the local resolution of the thin direction by scaling the local problem. We show eaxmples where the method is used both for geometry reconstruction [3] and for linear elastic deformation [2].

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Computing Deformations of 3D Elastic Bodies using the Meshless RBF-PUM method

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Key Words: Linear elasticity, partition of unity, radial basis functions, 3D deformation

In this talk we will present numerical simulations of deformed 3D objects. The simulations are produced by numerically solving the linear elasticity equations on complex shell geometries. We use the meshless RBF based partition of unity (RBF-PUM) method in the least squares formulation [1] and this talk will focus on applications of this method on various geometries.

The method is used to both reconstruct the geometries and numerically solve the governing PDEs. It is mesh-free and it solves the PDE in its strong form, pointwise. Hence, it is particularly adept in solving PDEs on complex geometries where mesh generation is non-trivial and the resulting mesh can be highly anisotropic. It is also easy to implement, flexible and computationally efficient.

The continuum bodies simulated are linearly elastic. We specifically assume small strains, meaning the constitutive relation between stress and deformation is linear. We compute the deformations by numerically solving a system of linear PDEs arising from Cauchy's equation of equilibrium in elastostatics. The deformed geometries include the Stanford Bunny [2], a hollow 3D cube with complex webbing and a 3D reconstructed model of the human diaphragm [3].

We will present realistic deformations and stresses, computed using the von Mises yield criterion. Finally, we will show convergence studies for the least squares residual and a comparison with the Finite Element Method (FEM) which proves that this method produces comparably accurate results. In conclusion, we aim to showcase the versatility and robustness of this method, especially when solving PDEs on complex 3D geometries.

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Discrete Conservation in Meshfree Collocation Methods for Fluid Flow

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Key Words: *Meshfree, Lagrangian, Conservation, Particles*

Over the last few decades, meshfree or meshless methods have become a popular alternative to conventional mesh-based solution procedures, especially for fluid flow problems with time-dependent domains and rapidly changing free surfaces. They can be easily used in a Lagrangian framework, which enables them to easily model large deformations and displacements. However, these advantages naturally come with their own challenges. One of the biggest drawbacks of meshfree methods is the lack of discrete conservation.

In this talk, we present an overview of different aspects of conservation issues in collocation-based meshfree methods. First, we discuss the lack of formal conservative properties inherent in the derivative approximation procedure across most, if not all, "purely" meshfree methods. Central to this is the lack of a discrete Gauss theorem, and the absence of a natural way to define fluxes. We show that obtaining formal conservation in this setting necessitates a global computation of discrete differential operators, which makes the solution procedure very slow and not feasible for Lagrangian frameworks. To avoid this, we introduce a method of approximate flux conservation in meshfree methods.

While focusing on incompressible flow, we also present the issue of volume and mass conservation in Lagrangian meshfree frameworks. We then introduce a concept of representative masses in Lagrangian meshfree collocation methods that can reduce the impact of these issues. We further introduce a notion of mass transfer between collocation "particles" that ensures the notion of representative masses can also be used for complex flow problems with large deformations in the fluid domain. After a series of verification and validation test cases that highlight the impact of the introduced framework, we also present the application of the method to an industrial test case of automotive water crossing.

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h-adaptive Radial Basis Function-Based Finite Difference Scheme for Boundary Value Problems of Linear Elasticity

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Key Words: Finite Difference Method, Radial Basis Functions, Polyharmonic Splines, Monomials, *h*-adaptivity, Linear Elasticity

In this research, an advanced finite difference (FD) scheme is constructed for the numerical solution of the partial differential equations (PDE) describing linear plane elasticity problems, which is based on the radial basis function technique (RBF). The widely-used RBFs are classified into two main groups, the infinitely- and the piecewise smooth RBFs [1]. The infinitely smooth RBFs depend on a shape parameter, setting the gradient of the RBFs and thereby controlling the condition number of the local RBF matrix, influencing the accuracy of the differentiation weights. However, the polyharmonic spline (PHS) as piecewise smooth RBF is independent of a shape parameter and its application can lead to higher convergence rates and more accurate results [1]. This is the reason why the PHS will be chosen for the computation of the weights. Furthermore, the PHS as RBF will be augmented with *p*-degree monomials for the sake of the achievement of faster convergence and increased accuracy.

An averaged residual-maxima based adaptive point-cloud refinement strategy will be presented and its computational performance will be tested on the convergence behavior of two kinds of benchmark problems: (i) smooth and (ii) non-smooth boundary value problems (BVP) (such as the shock- and the singular problem) [2, 3]. Since for these non-smooth BVPs, the *h*-adaptivity improves significantly the accuracy and the convergence rates, it would be worth extending the *h*-adaptive PHS-RBF FD method to 3D, time dependent and non-linear problems arising in solid mechanics.

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Meshfree GFDM for Elliptic Problems with Discontinuous Coefficients

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Key Words: Discontinuous Diffusion, GFDM, Anisotropic Diffusion, Meshfree

Physical properties with jumps appear in numerous applications in continuum mechanics such as multiphase flow, composite materials or phase change. Our goal is to describe phase change processes in a monolithic model with a meshfree generalized finite difference method (GFDM). Phase change leads to formation of interfaces at which physical properties such as thermal conductivity, density and viscosity have jumps. Since these physical properties appear in diffusion operators, we pay special attention to the formulation of the diffusion operator.

Meshfree GFDM have successfully been used in free surface flows with complex geometries. However, difficulties arise with the diffusion operator, since the method has no efficient way to ensure conservation of physical properties at interfaces or diagonally dominant numerical operators. This issue can be observed especially at interfaces where the diffusion coefficient has a jump, possibly of several orders of magnitude. Typical solution procedures for anisotropic laplacians include domain decompositions. However, in phase change we cannot predict the position of the interface and more importantly the interface can be smeared out accross a transition region.

To overcome the drawbacks of the current formulation, we present a numerical method that identifies regions where the diffusion coefficient has large jumps. A hybrid approach is proposed that ensures better algebraic properties for the linear system in these critical regions. This method is benchmarked against several test cases with varying jump magnitudes and geometric complexities of the interfaces.

Parameter Identification by Deep Learning for subsequent MESHFREE Simulations of Granular Media

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Key Words: *Parameter Identification, Meshfree method, Generalized Finite Difference Method (GFDM), Deep Learning, Inverse Problem, Model Reduction, Principal Component Analysis*

There are essentially two different paradigmatic approaches for mapping complex physical processes: classical physical modelling with associated numerical simulation (model-based) and prognostic methods based on the analysis of large amounts of data (data-driven). In recent years, the efficient combination of both approaches has become a research topic in its own right. However, research is far from an interlocking, problem-adapted application of these principles.

In the BMBF-project HYDAMO (Hybrid data-driven and model-based simulation of complex flow problems in the automotive industry), the interest is on the one hand in meshfree simulations of sand-like materials based on a model hierarchy with increasing complexity. The correct choice of parameters in the individual model stages is essential for the appropriate mapping of the processes. Furthermore, the development of an automated and efficiently calibrated prediction tool is necessary for industrial application. This is achieved by enhancements of the Generalized Finite Difference Method (GFDM) implemented in the MESHFREE software [1].

On the other hand, the project aims at reducing the high-dimensional parameters in a generic material model to their inherently nonlinear but low-dimensional structure by deep learning approaches and to identify them for the subsequent numerical simulation. As a step towards achieving this goal, data pairs generated from MESHFREE simulations (which solve the parametric partial differential equation (PDE) in a forward problem) are used to in turn apply deep learning methods for the parameter identification problem (inverse problem). Deep learning has recorded recent successes in solving parametric PDEs [2]. In this work, the method of interest here stems from the recent successes of deep learning, when combined with ideas from model reduction [3]. Here, stress over time constitutes the input, while the parameters of interest constitute the output. Both are reduced to some latent spaces by principal component analysis (PCA) and a neural network then maps these two latent spaces.

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Selection of sets of influence in meshless finite difference methods

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Key Words: *Meshless methods, meshfree methods, RBF-FD, GFDM*

I will present recent results on algorithms for stencil selection for RBF-FD and polynomial type meshless finite difference methods. The goal of these algorithms is to generate as small as possible sets of influence of desired accuracy, in order to maximize sparsity of the system matrix. The results are obtained in part jointly with Dang Thi Oanh, Ngo Manh Tuong, Mansour Safarpoor.

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Solving hyperelastic problems in biomechanics with least-squares RBF-FD methods

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Key Words: Radial basis functions, RBF-FD, least squares, hyperelasticity, biomechanics

Despite the flexibility of the collocation RBF-FD method to describe complex geometries and the simplicity of its implementation, the method has failed to gain significant traction in the solid mechanics community. This is at least in part caused by the fact that the method in its simplest form fails to give stable solutions for problems including Neumann boundary conditions and different stabilization techniques need to be used to include traction boundary conditions in the models.

However, recent research shows that problems with the stability can be overcome by oversampling the governing equation and solving the problem in least-squares sense [1]. This also allowed for an unfitted method to be developed, making it even simpler to describe complex geometries [2].

This contribution applies these new findings to the problem of hyperelastic solid mechanics models found in biomechanics with the purpose of modeling the human diaphragm [3]. The solution procedure is presented and the implementation is verified by comparison to FEM models. We perform a parametric study of the free parameters that are introduced by the solution procedure and the different evaluation paths that are made possible by the introduction of least squares solution to the governing equation.

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Stochastic flow simulation in 3D porous media, application the knee meniscus

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Key Words: Discretisation-Corrected Particle Strength Exchange, stochastic porous media, meniscus, data driven, homogenisation, Brinkman penalisation

Flow and transport computations for explicit microstructures of stochastic porous media, here the knee meniscus, are prohibitively time consuming. First, as the porous microstructure is geometrically complex, each simulation is considerably time consuming. Second, the porous microstructure is intrinsically stochastic as it varies from location to location and from specimen to specimen, requiring numerous time-consuming experiments and flow computations to be performed. First, we address the continuum biological hydrodynamics simulation in complex geometries, by presenting a novel integrated computational approach using the Discretisation-Corrected Particle Strength Exchange (DC PSE) [1] operator discretisation in a strong-form collocation mesh-less solver, the solver is coupled with Brinkman penalisation [2] to add a layer of robustness when dealing with such stochastic complex geometries. Steady and unsteady Navier-Stokes equations are solved using the solver. Then, we introduce a data driven framework in which the porous microstructures are homogenised to enable simulations in which the explicit microstructural representation is omitted, but the stochastic transport characteristics are preserved. Only a few meniscuses need to be characterised and a few sub- scale microstructural simulations on statistical volume elements are required to probabilistically identify the parameters of the random spatial fields of the permeability coefficient. The probabilistic identification setting assumes that each spatial input field is a realisation from a single, joint multi-dimensional probability density function. The probabilistic identification setting is based on Bayes' theorem, which only requires a limited number of measurements. Finally, we will use the identified probability density function to rapidly propagate the uncertainty with the fast homogenised model.

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Two-phase MESHFREE simulations with mass transfer model for free water surface evaporation

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Key Words: *Water, Evaporation, Meshfree method, Generalized Finite Difference Method (GFDM), Finite Pointset Method (FPM), Lagrangian, CFD, Multiphase, Multiphysics problems, Mass-transfer*

The evaporation of water can be easily observed in daily life. Unlike its occurrence, however, it is not straightforward to accurately resolve the problem and to predict the evaporation rate. Evaporation is a rather complex multiphysics mass-transferring process at the free surface between two phases — water and air, where a number of factors play roles [1]. Nevertheless, it is crucial to accurately estimate the evaporation rate at the given conditions in many industrial fields such as the prediction of local corrosion effects in automotive applications. Therefore, a robust numerical method is required to resolve evaporation phenomena.
The Finite Pointset Method (FPM), a Generalized Finite Difference Method (GFDM) implemented in the software MESHFREE, is widely used in academic and industrial areas [2,3], especially in automotive water management applications. Its efficiency is based on the meshfree character that eliminates the often-time-consuming process of meshing and re-meshing in other methods.
A mass transfer model is implemented in MESHFREE in order to simulate the free water surface evaporation phenomenon at the water-air interface. Thereby, it is assumed that the main driving force of the liquid mass transfer into vapour is diffusion driven by the vapour concentration gradient in the air phase close to the free water surface [4]. To resolve the vapour concentration gradient along the interface normal direction adequately, coupled two-phase simulations were executed. Hence, the simulation can also take into account the effects of forced convection and relative humidity in air phase, which are necessary to correctly predict the evaporation rate.
The simulation results are validated based on a series of experiments that measure the water evaporation rate with a relatively simple geometry. In the experiments, controllable conditions that highly influence the evaporation rate including air temperature, relative humidity and air flow rate are varied. The measured evaporation rates are then compared with the results from multiphase MESHFREE simulation with the newly implemented evaporation model.

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Unknown Parameter Identification from Noisy Training Data using Physics-Informed Neural Networks

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Key Words: *Physics-Informed Neural Networks, Deep Learning, Data-Driven Science*

Due to global warming and climate change, a number of natural disasters have been occurring in various places (e.g., the 2011 Tohoku earthquake and tsunami and the 2017 Northern Kyushu floods), raising the demand for predictive simulation technology. To perform numerical simulations, material parameters need to be determined, however, they depend on empirical laws and hence, their application ranges remain vague.

In this context, this work presents the application of Physics-Informed Neural Networks (PINNs) [1] to inverse problems of fluid flow. The characteristic of PINNs is that the network output is constrained to satisfy the informed physical laws, initial, or boundary conditions. This is achieved by forming the loss function as a linear combination of a supervised loss of data measurements and an unsupervised loss of governing equations by automatic differentiation [2] (Navier–Stokes equations in the presented study):

$$\mathcal{L} = w_{\text{data}}\mathcal{L}_{\text{data}} + w_{\text{PDE}}\mathcal{L}_{\text{PDE}} \tag{1}$$

$$\mathcal{L}_{\text{data}} = \frac{1}{N_{\text{data}}}\sum_{i}^{N_{\text{data}}} (\mathbf{u}_i - \hat{\mathbf{u}}_i)^2 + (p_i - \hat{p}_i)^2 \tag{2}$$

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_{\text{PDE}}}\sum_{i}^{N_{\text{PDE}}} (\nabla \cdot \hat{\mathbf{u}}_i)^2 + \left(\frac{D\hat{\mathbf{u}}_i}{Dt} + \frac{1}{\hat{\rho}}\nabla\hat{p}_i - \hat{\nu}\hat{\mathbf{u}}_i\right)^2 \tag{3}$$

Here, $\mathbf{u}_i$ and p_i are training data for velocity vector and pressure, $\hat{\mathbf{u}}_i = \hat{\mathbf{u}}(\mathbf{x}_i, t_i)$ and $\hat{p}_i = \hat{p}(\mathbf{x}_i, t_i)$ are PINNs-predicted velocity and pressure, respectively. $\hat{\rho}$ and $\hat{\nu}$ are identified density and kinematic viscosity of the fluid. Original work of PINNs [1] has investigated its applicability to slightly corrupted training data (1% noise), however, the data should have stronger noise in real-world applications. This work specifically considers its performance for inverse problems when the data includes 20% noise [3]. It further studies an approach to correctly estimate the unknown parameters ($\hat{\rho}$ and $\hat{\nu}$) by varying the weights to each of the loss terms and discusses PINNs applicability to considerably noisy training data.

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A comparison between Collocation and Galerkin Isogeometric approximation of acoustic wave problems

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Key Words: *Isogeometric Analysis, Collocation, Galerkin; Newmark methods; absorbing boundary conditions, acoustic waves.*

Isogeometric collocation methods combine the high smoothness of NURBS basis functions with the low computational cost of collocation methods, generating sparser stiffness and mass matrices than the ones generated by isogeometric Galerkin methods. Our previous work investigated the approximation of 2D acoustic wave problems with proper absorbing boundary conditions by Galerkin IGA methods in space and Newmark's explicit schemes in time (IGA-Gal-New). In this talk, we extend our study to IGA collocation explicit and implicit approximations (IGA-Col-New). A detailed numerical study on both Cartesian and NURBS domains illustrate the stability and convergence properties of the two Isogeometric Newmark methods with respect to the IGA and Newmark discretization's parameters. The experimental results show that the stability thresholds of the methods depend linearly on h and inversely on p, confirming that the proposed IGA-Col-New method retains the good convergence and stability properties of standard IGA-Gal-New and Spectral Element discretizations of acoustic problems.
Moreover, a detailed comparison of convergence errors, CPU time, and matrix sparsity patterns show that IGA-Col-New often outperforms IGA-Gal-New, in particular in the case of maximal regularity $k = p - 1$ and for increasing NURBS degree p. Some numerical results on the spectral properties of the IGA-Col-New matrices are also mentioned.

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A IETI Method for Trivariate Geometries with nonconforming Patches based on Mortaring

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Key Words: Isogeometric Analysis, IETI, Mortaring

In the simulation of real world problems using isogeometric analysis one challenge that often arises is the treatment of geometries with nonconforming discretizations of patches. One way to deal with these geometries is to make the patches conforming. This can be done manually or using suitable trivariate CAD software. However, for complex geometries it is not always possible to ensure compatibility of all trivariate patches at interfaces. In this case, a mortar method [1, 3] can be used to carry out simulation on nonconforming patches.

We present a workflow for the simulation of problems on 3D geometries with nonconforming geometry discretizations based on mortaring and IsogEometric Tearing and Interconnecting (IETI) method implemented in IRIT [2] and GeoPDEs [4]. For this method, we only require a pairwise matching discretization on the 2D interface of two neighboring patches for the numerical quadrature.

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Conforming/Non-Conforming Isogeometric de Rham Complex Discretization in Solid Toroidal Domains via Polar Splines

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Key Words: toroidal domains, polar splines, conforming/non-conforming Finite Element methods

We present a discretization of the continuous de Rham complex by means of adequate spline spaces sustaining the same cohomological structure, when the underlying physical domain is a toroidal solid. Discretizations preserving such homological invariant of the physical model are commonly exploited in electromagnetics to obtain numerical solutions satisfying important conservation laws at the discrete level. Thereby one avoids spurious behaviors and, on the contrary, improves accuracy and stability.

The toroidal geometries are of particular interest, for example, in the context of magnetically confined plasma simulations. The singularity of the parametrization of such physical domains demands the construction of suitable restricted spline spaces, called polar spline spaces, ensuring an acceptable smoothness to set up the discrete complex.

On the other hand, the polar structure of the basis functions is not compatible with parallel computing when adopting MPI algorithms, at least near the singularity. Whereas the tensor structure would easily accomplish the task. Therefore, in order to obtain a discretization capable to scale well with problems of large dimensions, we further present a, so called, conforming/non-conforming (CONGA) variation of the method. In this approach, the approximation is built in the ambient space of the tensor splines, which easily allows a parallelization of the processes, and then projected on the polar spline subspace to preserve the conformity of the discretization.

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Design-related Simulation – A Discussion

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Key Words: *Design-related simulation, Meshless finite elements, Topology optimization.*

The spread of simulation has changed the way how highly engineered products are designed. Finite element simulation made user friendly thru effective modeling software is the dominant technology for simulation. The introduction of optimization associated with finite element methods, especially generative design or topology optimization has transformed simulation into a design tool and moved simulation way up into the concept phase of design processes.

However, in many industries designer and analyst are separate functions. Management always wants designers to do analysis and simulation too. Skill levels are just different, and tools are not available to cater to a community that does not have the skill to make necessary assumptions that are needed to model complex events and systems with traditional means. Many attempts to create a simplified user experience to entice designers to adopt more simulation in their daily work did not change that. To a certain extend topology optimization packaged in an easy-to-learn user experience provided some part-level simulation capabilities to answer designer's simulation needs.

We will introduce a software solution that addresses the limitations above. This technology is completely meshless and works directly on CAD geometry. It can deal with assemblies and complex part connections in an easy way. Simplifications common in traditional mesh-based finite element methods (rigid elements for connections, thermal loads for bolt pretension, etc.) that require expert knowledge are not necessary. The software deals with the physics directly. Even the complicated task of figuring out boundary conditions for a part analysis becomes easy as complete assemblies can be dealt with.

We will discuss how this technology is going to change simulation processes. We will review the entire process chain of designing complex products, including the role of generative design, and how it interacts with design-related simulation.

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Efficient Numerical Integration for Trimmed Isogeometric Analysis based on Error Correction

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Key Words: isogeometric analysis, trimming, numerical integration, fictitious domain methods

The numerical integration on domains that are cut by an implicitly defined boundary curve or surface is an important problem that arises when solving partial differential equations on trimmed computational domains using isogeometric analysis or unfitted finite element methods. Since the assembly of the system matrices can be a bottleneck for the overall computation, efficient methods for the numerical integration are needed. At the same time, in order to guarantee optimal convergence orders, the method for numerical integration needs to achieve an approximation order that is equivalent to the approximation order of the employed discrete space.

In this talk, we present a method for the numerical integration on trimmed computational domains that is based on a local error correction approach. In each cut integration cell, we first find a linear approximation to the trimming boundary. Then, we increase the approximation order by adding correction terms based on a Taylor expansion. The computational complexity of the resulting method is equivalent to the complexity of a standard element-wise Gaussian quadrature on a non-trimmed domain.

In [1] and [2], we showed that the first order correction term results in a a fourth-order convergence rate in each cut integration cell and is therefore suited for isogeometric analysis with quadratic splines on both bivariate and trivariate domains. We generalized the method to obtain arbitrary approximation orders for numerical integration on trimmed planar domains in [3]. The method can therefore be used for high-order isogeometric analysis and for high-order unfitted finite element methods.

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Electromagnetic wave propagation through structure-preserving spline differential forms

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Key Words: Splines, Maxwell, Dual mesh, Hodge operator

A new *structure-preserving* numerical method will be presented which exhibits high order convergence and, contrarily to other high order geometric methods [1], does not rely on the geometric realization of any dual mesh. We use B-spline based de Rham complexes [2] to construct two exact sequences of discrete differential forms: the primal sequence $\{X_h^k\}$ starts from the space of tensor-product splines of degree p and at least C^1 continuity. The other spaces of the primal sequence are built by suitable tensor-product of splines of mixed degree p and $p-1$. Similarly, the dual sequence $\{\tilde{X}_h^k\}$ starts from the space of tensor-product splines of degree $p-1$, which in the parametric domain coincides with the last space of the primal sequence. The construction of the other spaces of the sequence follows an in the primal one, by using splines of mixed degrees $p-1$ and $p-2$.

The differential operators (gradient, curl and divergence) are comprised in the exterior derivative operator. Due to the high continuity of splines, the exterior derivative is well defined both for the primal and the dual sequence. Moreover, assuming vanishing boundary conditions on the primal sequence, the discrete spaces X_h^k and $\tilde{X}_h^{3-k}$ have equal dimension.

The method is completed with two sets of discrete Hodge–star operators, that relate the spaces of the two sequences, mapping the space of primal forms X_h^k into the space of dual forms $\tilde{X}_h^{3-k}$, and vice versa, for $k = 0,1,2,3$. The discrete Hodge–star operators encapsulate all the metric-dependent properties, including material properties. We will show a particular choice of the discrete Hodge–star operators inspired by [3] and how to compute them through the fast inversion of Kronecker product matrices. Finally, we will apply the method to the solution of Maxwell equations, and show that the method exhibits high order convergence and energy conservation.

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Explicit constants in isogeometric approximations

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Key Words: Isogeometric Analysis, Spline Approximation

Splines are piecewise polynomial functions that are glued together with a given smoothness. When using them in a numerical method, the availability of proper error estimates is of utmost importance. Classical error estimates for spline approximation are expressed in terms of (a) a certain power of the maximal grid spacing, (b) an appropriate derivative of the function to be approximated, and (c) a "constant" which is independent of the previous quantities but usually depends on the degree and smoothness of the spline.

An explicit expression of the constant in (c) is not always available in the literature, because it is a minor issue in most standard approximation analysis. There they are mainly interested in the approximation power of a spline space of fixed degree. However, one of the most interesting features in the field of Isogeometric Analysis is k-refinement, which denotes degree elevation with increasing interelement smoothness. The above mentioned error estimates are not sufficient to explain the benefits of approximation under k-refinement so long as it is not well understood how the constant in (c) behaves.

In this talk we extend the results of [1] by providing a priori error estimates with explicit constants for both the L^2-projection and Ritz-type projections onto spline spaces of arbitrary smoothness defined on arbitrary grids [2]. The presented error estimates indicate that smoother spline spaces exhibit better approximation per degree of freedom, even for low regularity of the function to be approximated. This is in complete agreement with the numerical evidence found in the literature.

We further discuss the extension of these results to the case of tensor product spline approximation and to isogeometric spline spaces generated by means of a mapped geometry, both in the single-patch and in the multi-patch case.

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Isogeometric Shape Derivatives for Maxwell's Eigenproblem

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Key Words: Isogeometric Analysis, Shape Morphing, Maxwell's Eigenproblem

In our work, we are investigating the Maxwell Eigenproblem in accelerator cavities whose performance is evaluated based on their eigenmodes. For cylindrical cavities, the eigenfrequencies and electromagnetic field distributions are known analytically and a well-known nomenclature is defined for classifying the modes. Due to the complex shape of real-world cavities, in practice the eigenmodes need to be determined using numerical simulations. Hence, also the classification of their eigenmodes is cumbersome.

Therefore, we investigate automatic mode recognition by deforming the cavity geometry to the cylindrical shape. To this end, an eigenvalue tracking technique is employed to ensure consistency of the solution along the deformation of the cavity geometry, i.e. to match the eigenpairs. Since crossings of the eigenvalues can occur along the deformation, sophisticated methods are necessary. Finally, the numerical results are aligned with the analytic solutions.

Employing Isogeometric Analysis (IGA) for the spacial discretization of the cavity allows for an exact representation of the geometry and smooth fields for subsequent particle tracking. Furthermore, describing the deformation of the geometry with IGA is straightforward and does not require remeshing along the shape morphing. In our work, we apply algorithms, which employ derivatives with respect to an introduced deformation parameter, to track the eigenvalues along the deformation. We formulate the required derivatives of the system matrices as shape derivatives with respect to the IGA control points.

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Leveraging code generation in numerical methods for complex geometries

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Key Words: Code generation, FEniCS, isogeometric analysis, immersogeometric analysis

Code generation for numerical partial differential equations (PDEs) lets users automatically compile efficient solver routines from mathematical problem descriptions. However, it typically assumes rigid code structures that are only immediately applicable to certain numerical methods, such as the finite element (FE) methods considered in the FEniCS [1] code generation system. Standard FE methods cannot be applied directly to PDE systems on geometries from typical computer aided design (CAD) systems; they also struggle with geometric complexity arising from nonlinear physical phenomena, e.g., extreme deformations, contact, or fracture. Numerical schemes to couple non-matching parameterizations of geometry or handle large deformations and topological changes cannot be directly implemented using FEniCS's standard code generation workflow. Thus, an active area of research is: How can advanced code generation capabilities be productively applied in such methods? The present talk will review how FEniCS has been extended to isogeometric analysis [2] and discuss a recent extension to shell analysis of aerospace structures defined using multiple non-matching spline patches [3]. We will also discuss advances in fluid–structure interaction (FSI) analysis using CAD-based descriptions of thin structures immersed in unfitted meshes, building on preliminary work from [4]. This will enable rapid prototyping of both constitutive and geometric modeling choices in the design and FSI analysis of prosthetic heart valves. Lastly, we will cover ongoing work toward leveraging code generation within a general-purpose framework for high-order immersed finite element and isogeometric methods. These various projects illustrate different promising approaches to the central research question identified above.

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On the Accuracy and Efficacy of IGA-BEM Solvers for 3D Lifting Flows

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Key Words: *Isogeometric Analysis, 3D potential flow, Adaptive Refinement*

The authors have previously presented in [1] the development and benchmarking of an IsoGeometric Analysis Boundary Element Method (IGA-BEM) solver for the 3D flow around lifting wings with finite span, based on Morino's formulation for the perturbation potential [2]. The solver employs the same analysis-suitable T-spline basis for the representation of both wing's boundary surface and the unknown field quantities. The 3D character of the flow near the wing tip and the resulting flow velocity singularity at the intersection of the wing tip with the trailing edge entail the adoption of a local refinement process to improve the rate of convergence of the numerical solution of the problem.
In this work, we are focusing on the study of the accuracy and efficacy of the original IGA-BEM solver using both NURBS and T-splines representations for the body geometries. Specifically, we are interested in:

1) the efficacy and achievable accuracy of different global and local refinement strategies when evaluating the quantities of interest (pressure & lift). Our strategies include standard adaptive refinement schemes comparing successive refinement steps, and a simplified refinement approach which compares the values of the solution at neighboring collocation points and refines the corresponding knot intervals when differences are larger than a specified tolerance.
2) The efficacy and accuracy that can be achieved by optimizing the methods of integration and the number of quadrature points used in the calculation of integrals involved in the assembly of the matrix of the employed collocation scheme.

Results and comparisons employ both NURBS and T-Splines geometry representations.

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Strengthening the Predictivity of Numerical Design in Production Engineering with CAD-Based Discretisation Methods

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Key Words: *Inverse Design, Shape Optimization, Production Engineering*

Without appropriate manufacturing processes, product innovations cannot be brought into our daily lives. As such, there is a constant need for innovative, flexible, and precise manufacturing processes. At the same time, the manufacturing process can act as a significant cost driver, in particular in the range of small lot sizes. These costs can be divided into two categories: One is the manufacturing step itself, which requires material and tailored machinery. The other category is the design of the manufacturing process, a preprocessing task that defines tool shapes, plans paths, etc.. This presentation is concerned with improving the design step of manufacturing both in terms of accuracy and efficiency.

Already for several decades now, the design of manufacturing processes has profited from numerical simulation methods. These methods were, and are still, used in order to facilitate the iterative design process. Instead of having to test each preliminary design directly in the manufacturing process, it is much more cost- and time-efficient to run these tests in a simulation environment. Furthermore, in more recent years, inverse design methods have gained traction in the field. These methods design the manufacturing process based on the desired product outcome with little to no intervention by the design engineer.

In particular the inverse methods profit immensely from CAD-compatiblity, allowing to tightly interlace these methods with the CAD/CAM process. Exemplified via the manufacturing processes of injection moulding [1] and metal cutting [2], we will demonstrate how CAD-based methods not only improve the integration into the overall design process, but also possess superior properties in terms of accuracy and efficiency.

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Tailoring a mesh generator for 3D NEFEM to avoid de–featuring

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Key Words: exact geometry, NURBS–enhanced FEM, de–featuring, mesh generation

Contemporary industrial design requires building computer aided engineering (CAE) models suitable for simulation. This task is known to be a major bottleneck due to the excessive human intervention required when processing the upstream computer aided design (CAD) model. In general, generating meshes from a complex CAD model largely depends on the type of simulation, because of the numerous multiscale features which may or may not be negligible for the physical problem of interest. Traditional mesh generators produce small, often distorted, elements, when the mesh size desired by the problem exceeds the dimension of the geometric features. Large research efforts have been made into methods of de–featuring complex CAD models. However, fully automatised de–featuring has not yet been achieved. Firstly, it is not always possible to know in advance the effect of the de–featuring before actually performing simulations. Secondly, the de–featuring requirements differ from problem to problem, due to their physical nature. Finally, de–featuring also relies on the desired approximation level.

The NURBS–enhanced finite element method (NEFEM) circumvents this problem, through a complete separation of the geometric representation from solution approximation. The two concepts have been tightly coupled in the large majority of available solvers through the isoparametric concept. Within NEFEM, the geometric description uses the boundary representation (B–rep) information directly from the CAD model in the parameter spaces, whereas polynomial functions are used to approximate the solution in the physical space. This new paradigm avoids the need for de–featuring. In addition, the method allows discretisation of the CAD model with a mesh size that respects the user specification and is not restricted by the presence of small geometric features.

This work will present a new mesh generation technique, in which element faces may span across multiple surfaces and retain the exact B–rep. The mesh generation process will be detailed, including the new quality metrics that have been devised specifically for the NEFEM elements. Several examples will be presented to demonstrate the potential of the proposed technique.

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Adaptive smoothing Newton methods based on primal-dual gap estimators

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Key Words: Inexact Newton methods, Non-smooth minimzation, A posteriori error estimation

The convergence of the standard Newton algorithm hinges on the smoothness of the target nonlinear system. There is a wide class of modified Newton algorithms that address the case where the standard method fails due to low regularity. In particular, we consider so-called smoothing Newton methods [4] where non-differentiable functions are replaced by smooth approximate counterparts. The amount of smoothing is proportional to a parameter that should decrease as the smoothed iterations progress.

We seek a criteria for the smoothing parameter using a posteriori error estimation. We consider PDEs arising from the minimization of a non-smooth energy functional. Thus, we may use a so-called primal-dual gap estimator. The estimator measures the error in a computed solution by invoking a dual maximization problem. In particular, the estimator provides a constant-free upper bound for the difference of the energy of the true and computed solutions.

This strategy has been applied recently to non-smooth minimization problems in [1], where the primal and dual problems are solved in a globally coupled manner and no smoothing is used. In this talk, we instead present a patchwise-local and decoupled solution of the dual problem [2, 3] and use a smoothing Newton method for solving the primal problem. We also compute estimators that target the smoothing, linearization, and discretization components of the overall error in the smoothed problems. This leads to an adaptive algorithm steering the mutual sizes of the components as in [3].

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An Efficient Mixed FE-Formulation for Gradient Elasticity at Finite Strains

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Key Words: Mixed Finite Elements, Gradient Elasticity, Finite Element Discretization, Finite Strains

Gradient elasticity formulations enable the modeling of size effects, which appear when the scale of material heterogenities approaches the scale of the macroscopic mechanical fields. Furthermore, due to the higher regularity of the solution, corresponding numerical simulations remain mesh-independent, since they are free of geometry-induced nonphysical singularities, which appear in local models at e.g. sharp corners or crack tips of the modeled specimen. Since gradient elasticity models incorporate second-order deformation gradients, purely displacement-based finite elements require C^1-continuity, for which unstructured meshing and retaining compatibility with standard software are known challenges. Another approach is to introduce displacement gradients as separate discretization variable. Corresponding mixed FE-formulations require only to be C^0-continuous and thus, standard interpolation with piecewise polynomial functions is sufficient. However, due to the introduction of additional variables, the development of corresponding numerical schemes which are cost efficient, stable and robust, is essential. Here, a formulation is presented, in which similar to an approach proposed in [1] the internal elastic potential is formulated exclusively in terms of the displacement gradient variable. A constraint term incorporating a divergence-free Lagrange multiplier enforces the rotation part of the gradient variable to vanish, which is a necessary condition for gradient fields. In a second constraint term the divergence-free condition is enforced. The corresponding discretization follows the approach of [2], which enables static condensation of the first Lagrange multiplier and thus, keeping the number of degrees of freedom at a minimum, while maintaining suitable mathematical solution spaces. Moreover, as shown in [2], the discrete Lagrange multipliers corresponding to the second constraint are identified as an approximation of the displacement solution. Thereby, displacement boundary conditions can be incorporated directly avoiding the necessity of a pre- and postprocessing step (cf. [1]). In a displacement-driven numerical test on a domain with hole and non-connected boundary convergence is shown. Other numerical tests further show robustness for varying nonlocal constitutive parameters and increased computational efficiency compared to other mixed approaches (c.f. [1, 3]).

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Artificial instabilities in finite element analysis of large deformation elasticity problems and a strategy to avoid them

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Key Words: *Mixed Finite Elements, Nonlinear Elasticity, Stability, Hourglassing.*

This contribution addresses the issue of artificial instabilities in discrete solutions obtained by various non-linear finite element formulations (cf. [2]) occurring under homogeneous stress states in elasticity problems. While avoiding locking is crucial for accurately capturing physical instabilities, it is often observed that some locking-free formulations suffer from artificial, non-physical instabilities, usually referred to as hourglassing (cf. [1], [3]).

Analytical stability analyses of simple reference problems are presented and compared to the discrete solutions. This allows assessing precisely the performance of various finite element formulations for a broad range of input data, e.g. element aspect ratio and elastic constants. The sources of the hourglass phenomena triggered by compressive and tensile stress states are highlighted and, on this basis, a simple strategy to construct stable and locking-free finite element formulations is proposed.

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Convergent Approximations to Global Minima of Integral Functionals using Polynomial Optimization and Finite Element Methods

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Key Words: finite element methods, global nonlinear analysis, sparse polynomial optimization, Gamma convergence, sum-of-squares relaxations

Computation of minima of nonlinear integral functionals (e.g. strain energy) is typically done by using a variation of Newton's method or a gradient descent method on the Euler-Lagrange PDEs associated to the functional. However, these procedures only guarantee finding an approximation to a local minimum, but say nothing of whether the solution is a global minimum of the functional, which often is the goal. Finding an algorithm that provably converges to a global minimum is a classical and fundamental challenge in many fields, including nonlinear elasticity, fluid mechanics, pattern formation and PDE analysis. In this work, we leverage theoretical tools from the fields of sparse polynomial optimization (within algebraic geometry) and finite element (FE) methods to present such an algorithm. The techniques include exploiting properties of sparse sum-of-squares (SOS) relaxations and Gamma convergence to prove convergence to a global minimum of a functional with a polynomial integrand as the mesh is refined and the moment-SOS relaxation order is raised. We present numerical examples which result in excellent approximations to the global minima of different nonlinear functionals, including the pattern-forming Swift-Hohenberg free energy in two spatial dimensions, even when one uses sparse SOS relaxations that are computationally cheaper, but lack convergence guarantees. Finally, we also outline how to extend these methods to PDE-constrained optimization problems and show some preliminary results in this context.

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Dynamics and Locking of Shell Eigenmodes

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Key Words: Shells, Locking, Asymptotic Analysis, *p*-Version

Shell structures have a rich set of features resulting from the interaction of the shell geometry and the deterministic parameter, the thickness of the shell, which is often modelled as a dimensionless quantity. In this talk the connection between the boundary layers (including the internal ones) and the smallest eigenmodes is discussed.

For shells of revolution the asymptotics of the smallest eigenmodes have been analysed by various authors and with the exception of some corner cases the overall behaviour is well understood [1],[2]. What is new here is that the the asymptotic convergence rates for the eigenmodes are shown to be tied directly to those of the corresponding internal boundary layers. Spatial resolution of the boundary layers in FEM is known to give rise numerical locking or loss of optimal convergence rate – in this case eigenlocking. Even in the case of eigenlocking, the individual modes converge at the predicted rate, but they appear out-of-order due to error amplification manifested in constants.

The numerical experiments cover all major shell geometries and a practical range of dimensionless thicknesses.

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Hourglassing-Free Petrov Galerkin Enhanced Assumed Strain Finite Elements Insensitive to Mesh-Distortion for Nonlinear Solid Mechanics

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Key Words: enhanced assumed strain, Petrov-Galerkin, mesh-distortion sensitivity, hourglassing-free

The enhanced assumed strain (EAS) method proposed by Simo et al. [5] is one the most successful mixed finite element methods. Despite its success and numerous improvements there are still some open issues. Two of which concern mesh-distortion sensitivity and hourglassing-instabilities.

MacNeal [2] has shown that the optimal element performance cannot be achieved with a symmetric stiffness matrix. This lead to a Petrov-Galerkin approach termed unsymmetric finite element method which effectively allows construction of mesh-distortion insensitive high order finite elements [4]. However, unsymmetric low-order elements are often complex, require many internal degrees of freedom or a priori knowledge of the material model [6, 1]. Recently, Pfefferkorn and Betsch [3] proposed a Petrov-Galerkin approach based on the EAS method which overcomes these drawbacks and allows a simple construction of high performance low-order elements.

The present contribution concerns the extension of this method to nonlinear hyperelastic and elastoplastic problems. Focus is put on an hourglassing free formulation which could be achieved by enhancing the spatial displacement gradient instead of the usual enhancement of the deformation gradient.

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Locking behaviour in linear and nonlinear analysis: an application to the flat and curved version of the T6-3i shell finite element

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Key Words: Shear and membrane locking, T6-3i finite element, geometrically exact shell theory.

Since the pioneering works of Argyris in the parametrization of finite rotations, several alternatives to formulate a genuine geometrically exact shell theory have been devised. In general, the only way to tackle the problems resulting from such theories is the finite element method. However, conventional displacement-based finite elements tend to deliver a poor performance as the slenderness of such structures increase. Assumed Natural Strain (ANS) and Enchanced Assumed Strain (EAS) techniques are often used to alleviate the unbalance of the shape functions in reproducing certain limiting conditions.

In the present work the authors study the behaviour of the T6-3i triangular finite element [1, 2]. This surprisingly *simple* element is advantageous from the implementation point of view, as its elemental computations are extremely fast to perform. However, the fact that its rotation field is non-conforming raises concerns on its ability to always converge to the exact solution. Moreover, although its displacement field was designed to satisfy the Kirchhoff limit constraint (at least for linear analysis *shear-locking* is absent), its membrane behaviour does not satisfy the limit constraints when the element is curved.

The aim of the authors is to assess the behaviour of the element under varying thickness values. Linear *versus* nonlinear analysis are performed for both *flat* and *curved* geometries. It is shown that the type of analysis (linear *versus* nonlinear) has a strong influence on the quality of the results. Unlike linear analysis, in non-linear regime there is always a coupling between bending and membrane behaviour (even in the case of flat elements).

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Nonlinear Poisson Stiffening Effects in 3d-shell Models

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Key Words: *3d-shell model, Poisson stiffening, locking*

In recent years, there have been many developments in the field of 3d-shell models. Compared to standard shell models, 3d-shell models allow for thickness change [1]. When simulating with only one layer of elements across the thickness, it has proven important to include linear transverse normal strain into 3d-shell models to avoid a stiffening phenomenon, often referred to as Poisson thickness locking. This is done either using the EAS-method [2] or by a quadratic displacement field in thickness direction [3].

When simulating bending over small radii using certain 3d-shell finite elements in LS-DYNA, Fleischer [4] observed an additional stiffening effect, which remained unexplained so far. In case of large strain, the elements behave remarkably stiffer than a converged numerical reference solution, although measures to avoid Poisson thickness locking are included.

This contribution focuses on the explanation of the stiffening effect described above. The stiffening effect turns out to be of higher order, which means that it is present only in case of large deformations in geometrically nonlinear simulations. Furthermore, a method to avoid the stiffening effect is derived and its feasibility is confirmed by numerical results.

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Quantitative Evaluation of Shear Stiffness on Nonlinear, Linear and Two Intermediate Degrees of Partly Nonlinear Strain in 3D Membrane Theory and 2D Disc Theory for the 9-Node-4-Corner Finite Element

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Abstract

3D nonlinear membrane theory is assumed by 2nd Piola-Kirchhoff stress tensor and Green-Langrange strain tensor or by Cauchy stress tensor and Euler-Almansi strain tensor. The governing partial differential equation for 3D dynamic in-plane tensile force equilibrium considers second-order spatial derivatives of 3D displacement. The 9-node-4-corner finite element with biquadratic interpolation functions on nodal undisplaced 3D coordinate in stress-free state and on nodal 3D displacement is applied for spatial discretization within 3D nonlinear membrane theory (static equilibrium; dynamic equilibrium) – that for 2D plane geometry and in-plane 2D displacement includes and represents 2D nonlinear disc theory – . Geometric element height-width ratios that deviate strongly from unit value one induce nonlinearly increasing element shear stiffness by linearly increasing element height-width ratio. The 2D plane case of the 9-node-4-corder finite element with unit element height two units of length and parameter varying width from 0.1 to 10 units of length is exposed to parameter varying static in-plane 2D boundary shear displacement from small strain inducing 0.01 units of length to large strain inducing 10 units of length. Since element shear stiffnesses for assumptions of nonlinear strain and linear strain differ from each other and for assumption of nonlinear strain shear stiffness highly nonlinearly increases with increasing element height-width ratio furthermore two different intermediate degrees of partly nonlinear strain are considered for evaluation. Comparison between element shear stiffnesses by assumptions nonlinear, linear and two intermediate partly nonlinear strains is drawn for the above parameter ranges. Appropriate approximation of nonlinear strain by linear strain and two intermediate partly nonlinear strains, respectively, is concluded for high element height-width ratios to keep element shear stiffness realistic, representative and practical within 3D curved geometries for 3D membrane (static and dynamic) computations by application of the 9-node-4-corner finite element. Comparison focuses on element shear stiffness itself, applied increment factor within equilibrium iterations until convergence and number of equilibrium iterations until convergence.

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Unconditionally stable dynamic analysis of multi-patch Kirchhoff-Love shells in large deformations

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Key Words: Nonlinear dynamics; Large deformation; Stability; Kirchhoff-Love; Multi-body; Shells

One-step implicit time integration methods such as Newmark's schemes are only conditionally stable when used in large deformation analyses [1]. Simo and Tarnow proposed a simple method that guarantees unconditional stability by conserving the algorithmic energy in elastodynamics [2]. However, energy conservation is lost for other structural models as the Kirchhoff-Love theory, more efficient in the terms of spatial DOFs for thin shell problems, where the strain-displacement relationship is no longer quadratic. This work presents a numerical framework for long term dynamic simulations of structures made of multiple thin shells undergoing large deformations. The C1-continuity requirement of the Kirchhoff-Love theory is met in the interior of patches by cubic NURBS approximation functions, according to the isogeometric concept, with membrane locking avoided by patch-wise reduced integration [3]. A simple penalty approach for coupling adjacent patches, applicable to either smooth or non-smooth interfaces and either matching or non-matching discretizations is adopted to impose translational and rotational continuity [4]. The time-stepping scheme of Simo and Tarnow is generalized to achieve energy conservation for generally nonlinear strain measures and penalty coupling terms, like the nonlinear rotational one for thin shells. The method is based on a particular integral mean of the internal forces over the step, that includes Simo and Tarnow's method as a reduced quadrature rule, and has unconditional stability.

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Computation of Incompressible Flows on Adaptive Unit Curvilinear Grids

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Key Words: Mesh adaptation, Mesh generation, High-order mesh, Interpolation error, Quasi-unit mesh

A significant part of recent research in mesh generation has been devoted to the generation of body-fitted curvilinear meshes. Curved elements on the boundaries mitigate the error caused by the approximation of curved geometries by straight-sided meshes. The natural extension of the use of curvilinear meshes is high-order mesh adaptation. Here, we propose a methodology aimed at the generation and adaptation of two dimensional curvilinear anisotropic meshes. The quadratic triangular elements follow the features of a numerical solution computed e.g. with the finite element method, allowing a reduced number of degrees of freedom for a comparable interpolation error. The metric tensor field used to generate the elements is defined based on an interpolation error estimate, using recovered derivatives of order up to three of the numerical solution. A quasi-unit straight-sided mesh is first generated by spawning points in the computational domain in such a way that two neighbouring points lie within the range of $[1/\sqrt{2}, \sqrt{2}]$ when computing distances with respect to the metric field, then by connecting them using a standard anisotropic mesh generator. Straight-sided edges are then curved by moving the mid-edge nodes to approximate the geodesic between the edges's extremities while ensuring the validity of the elements at all time. Topological operations such as curvilinear edge swaps and curvilinear small polygon reconnection (CSPR) are finally applied to the curved triangulation to further increase mesh quality, yielding a quasi-unit curved mesh with only valid elements. For a comparable complexity, adapted meshes exhibit a reduced interpolation error compared to straight-sided anisotropic meshes. Numerical applications, such as tracer advection and Von Kármán streets, are presented to illustrate the method.

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Optimization, Adaptivity, and Surface Fitting of High-Order Meshes

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Key Words: Mesh Optimization, High-Order Methods, Finite Elements, Adaptivity

We present a framework for adaptive optimization of high-order curved meshes. The optimization process is driven by information that is provided by the simulation in which the optimized mesh is being used [1]. We make the important choice to require only discrete description of the simulation feature to which to adapt to, e.g., the feature can be described as a finite element function on the mesh. This is a critical step for the practical applicability of the algorithms we propose and distinguishes us from approaches that require analytical information.

The discrete problem is formulated as a variational minimization of a chosen mesh-quality metric, utilizing a finite element extension to the Target-Matrix Optimization Paradigm [2]. The method primarily relies on node movement (r-adaptivity), but also has the capability to perform h-adaptivity steps when this can produce to the desired local mesh size [3]. We will also discuss our latest capabilities for surface fitting and tangential relaxation, which are enforced weakly by adding penalty terms in the objective [4]. These penalty terms connect the concept of mesh motion to the discrete finite element function that defines the desired node position.

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Dragged Solids: Three-dimensional Solids with the Kinematics of Geometrically Exact Models

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Key Words: Structural models, reduced model, geometrically exact rod and shell, contact.

One of the main challenges that structural models face, both from theoretical as well as from the numerical standpoints, is their incorporation into continuum models. This is so because, while some problems are purely structural, many relevant problems in engineering and mechanics cannot be adequately represented only with reduced dimension models but greatly benefit from incorporating them as part of the physical model. For example, while a cable might be represented with enough accuracy using a string or a bar model, its anchorage onto a bridge pillar might require a full three-dimensional model if a faithful representation of the stresses is required. Connecting these two descriptions is far from trivial.

Among this kind of problems, maybe the most important class involves interactions between reduced order models and continua. In particular, fluid/structure interactions between such bodies are notably difficult and have only been partially resolved before. The interaction between a fluid and surfaces such as the ones of flags, parachutes, sails are complex to model, but even more with cables and beams.

Based on our recent work [1], we will present a methodology for the formulation of solids with the kinematics of geometrically exact rods and shells. By a variationally consistent procedure, the motion of points in these bodies is dragged by a structural theory, while the interactions (surface and body forces) are resolved at the continuum level, with full accuracy. The outcomes of this approach are slender bodies (rod-like, shell-like), with very few degrees of freedom that can be used with standard contact and interaction solvers, and combined with full 3D solids without add hoc interfaces.

Exploiting the ideas of the model projection and kinematic lifting, one obtains, if desired, exact rod and shell models that use three-dimensional material constitutive laws. With this, and without any constitutive projection, elastic *and* inelastic constitutive laws can be used in the context of reduced order theories.

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Fluid-structure interaction of slender bodies immersed in three-dimensional flows: a new approach for mathematical modeling and numerical approximation

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Key Words: *fluid-structure interaction, beam theory, mixed dimensional PDEs*

For the computational analysis of slender structures, one-dimensional (1D) models are commonly used to reduce the computational cost of simulations. However, the coupling of three-dimensional (3D) continua with immersed 1D structures is not yet well investigated from the mathematical and computational standpoint, although it arises in applications of paramount importance such as biology, biomedical engineering, geoscience and the mechanics of reinforced materials. We leverage on a new framework to formulate and approximate coupled partial differential equations (PDEs) on manifolds with heterogeneous dimensionality [1,2,3]. On the basis of this theoretical knowledge, we study the mathematical formulation and develop numerical methods for fluid-structure interaction (FSI) that combine a 1D representation of the slender structure with a 3D formulation of the flow. It is known that 3D-1D coupled problems can be interpreted as 3D problems with concentrated sources (Dirac deltas) located on lower dimensional manifolds of the domain [4]. The solutions of such problems are affected by low regularity, which in turn reduces the ability to construct convergent and efficient approximation methods. The new approach that we propose overcomes the previous issue because it has the fundamental advantage to enable the approximation of the problem using Galerkin projections on Hilbert spaces [1,2,3]. For this reason, we are able to perform a rigorous convergence analysis of approximation methods, such as the Finite Element Method (FEM), applied to these problems [1,2]. First, we address some general aspects of 3D-1D mixed dimensional PDEs, with particular attention to their coupling, achieved by means of Lagrange multipliers combined with a suitable projection operator form the 3D solution space to the 1D space [3,5]. Second, we apply this approach to the case of the interaction between a beam and an incompressible fluid, described as a 3D-1D FSI problem. In this case, we compare different coupling strategies, putting into evidence the advantages of the proposed approach.

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How Well Do Constraint Mixture Models Represent Fibrous Soft Tissues? A Comparison Against Embedded, Discrete Fiber Models

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Key Words: *Fibrous Soft Tissues, Embedded Fiber Networks, Timoshenko-Beam, Beam-to-Solid Coupling*

Fibrous soft tissue such as collagenous connective tissue or blood clot may be thought of as fiber network embedded in a homogeneous solid matrix, i.e., “ground substance” [1]. Models of these tissues are important to our understanding of their fundamental structure-function (or -dysfunction) relationship. In the past, various modelling approaches have been taken that spanned all the way from simplified continuum approaches up to a complete spatial modelling of the area-to-volume fiber-matrix interface [2]. Which begs the question: what is the exact trade-off between accurate description of the macroscale behaviour and model complexity? To answer this question, we developed models of the elastic, coupled bulk-fiber behaviour of fibrous soft tissues representing two distinct levels of model complexity. We compared their performance under three naturally occurring deformation modes, namely uniaxial extension, simple shear, and pure shear.

First, we develop a low-fidelity model, with a continuum approach of the fibrous tissue as an incompressible, anisotropic, hyperelastic material. This approach accounts for the fibrous structure in the strain energy function through a continuous probability density function of the fiber orientation. At the deformed configuration, the contribution of the fibers is spatially integrated over a unit sphere domain, as in the work by H. Chieh and G. Ateshian [3]. Next, as our high-fidelity model, we consider an embedded discrete fiber network into a hyperelastic solid matrix. We model each fiber as a spatial Timoshenko beam. Next, we couple the translational degrees of freedom of the beam’s centerline to the displacements of the solid matrix through a Lagrange multiplier field, as proposed in the mortar-type finite element method by Steinbrecher et al. [2]. Specifically, we implement the segment-based integration of coupling elements of initially curved beam networks and conduct proper consistency and convergence tests by developing a user subroutine on the commercial code Abaqus/Standard.

Using both approaches we will consider a representative volume element with one dispersed principle fiber bundle (single fiber family). We will investigate and report the ability of our high-fidelity model (embedded fiber network) to accurately capture the (de-) coupled behaviour of the fiber network and the solid matrix. Furthermore, we will particularly focus on the trade-off between model complexity and computational cost with respect to practical, experimental aspects of soft tissues mechanical testing under large deformation.

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Linear and nonlinear 1D-3D models for fluid exchange between tubular networks embedded in porous media

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Key Words: *mixed-dimension method, embedded networks, 1d-3d coupling, root water uptake, tissue perfusion, smoothing kernel*

Mixed-dimension 1D-3D methods allow to efficiently describe systems tubular networks embedded in porous media where fluid is exchanged between network and the porous bulk and dominates the fluid distribution in the porous medium. Two examples of such systems are fluid flow in microvasculature and embedding tissue [1], and water uptake of plant roots from soil [2]. Due to the nature of thin inclusion fluid pressure profiles in the porous bulk usually exhibit large gradients in the vicinity of the inclusion and pose difficulties for numerical schemes approximating pressure profiles and fluid flow. For example, particularly for dry soils local water pressure gradients can be become very large in the vicinity of roots due to the nonlinear relationships of water saturation, water pressure and soil permeability. Commonly used discretization lengths (for example 1cm) in root-soil interaction models do not allow to capture these gradients accurately.
We present a numerical scheme targeted at resolving such issues. The numerical scheme combines smooth distribution functions in the vicinity of the network with interface reconstruction schemes based on local analytical solutions. We explore accuracy and limitations of the scheme in numerical test cases. We present the results of a recently published benchmark case and present the latest results regarding time-dependent problems of water uptake from soil or exchange of small molecules between microcirculation and embedding tissue.

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On Solution Methods for Multiphysics Problems in Brain Biomechanics

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Key Words: *Multiphysics Problems, Mixed-dimensional models, Solvers, Preconditioning, Fractional Laplacian operator*

We are interested in reliable simulations of biophysical processes in the brain, such as blood flow and metabolic waste clearance. Modeling those processes results in interface-driven multiphysics problems that can be coupled across dimensions. The coupling is imposed by the Lagrange multiplier that enforces constraints on the interface and ensures well-posedness in fractional Sobolev spaces weighted by material parameters. However, the complexity of the interface coupling often deteriorates the performance of standard methods to finding the numerical solution.

Therefore, we derive preconditioners and solution techniques which target specifically such multiphysics problems by exploiting fractional operators at the interfaces for order optimal performance. Specifically, the robust preconditioners for the interface problems are represented as a sum of fractional Laplacians that can include both negative and positive fractionalities. To handle fractional operators numerically, we implement methods based on multilevel algorithms and rational approximation. We show that the numerical methods are parameter-independent and scalable with regards to number of the degrees of freedom of the system. We demonstrate the efficiency of our methods on several numerical examples of mixed-dimensional problems on realistic geometries, such as 3D-1D model of flow in vascularized brain tissue.

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Parameter-robust Methods for the Biot-Stokes and Darcy-Stokes Interfacial Coupling without Lagrange Multipliers

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Key Words: Robust solvers, operator preconditioning, Biot-Stokes coupling, Darcy-Stokes coupling, Perturbed saddle-point problems

Coupled multiphysics mixed-dimensional systems pose a special challenge for construction of solution algorithms which should remain efficient accross a wide range of model parameters typically found in the applications. It is known that if the coupling variable/Lagrange multiplier is explicit in the problem formulation such algorithms often require fractional order operators on the interface. In this work we consider formulations of the coupled Biot/Darcy-Stokes problems (solved for Biot displacement-total pressure-fluid pressure/Darcy pressure and Stokes velocity-pressure) which are free of Lagrange multipliers. We first show that sub-physics preconditioners are stable only in certain parameter regimes. Then, using an abstract theoretical framework we construct mesh-independent and parameter-robust monolithic preconditioners for both problems. A critical component enabling robustness are the appropriately weighted operators in fractional Sobolev and metric spaces at the interface. Several numerical examples using finite element and finite volume methods will be presented demonstrating performance of the proposed preconditioners.

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Anisotropic Extension of a Model for Ferroelectric Materials with Ferroelectric to Antiferroelectric Phase Transformation

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Key Words: *Ferroelectric material models, anisotropic, polarization*

The FE-AFE Ceramic material model in the ALEGRA finite element code has traditionally been used to model inelastic strain and polarization changes of ferroelectric materials undergoing ferroelectric (FE) to antiferroelectric (AFE) phase transformations. However, this model has been shown to be insufficiently general under anisotropic (non-hydrostatic) stress loading.

An extension to this model based on a different transformation strain mechanism at the crystal scale was proposed based on an analysis of crystallographic data. This model extension was implemented as a proof of concept in Python [1], and the resulting simulations show significant improvement in agreement with experimental data.

In this talk, we will describe the FE-AFE Ceramic material model and show the limitations of the old approach, in which the transformation criterion and inelastic transformation strain for a domain depends on the orientation of the dipole vector. We will then describe the new approach, in which both dipole and crystal orientations are considered, and show that better agreement with experimental results is achieved with this new approach.

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Microstructure-Explicit Simulation of Electromechanically-Driven Dielectric Breakdown of P(VDF-TrFE)/nAl Films under Impact Loads

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Keywords: *Energetic materials; Piezoelectricity; Flexoelectricity; Dielectric breakdown.*

Materials such as poly(vinylidene fluoride-co-trifluoroethylene), or P(VDF-TrFE), are known to exhibit piezoelectric and flexoelectric behaviors. While numerous studies have been performed to predict the conditions under which chemical reactions initiate (ignition threshold) as a result of thermal and mechanical dissipation mechanisms, there is a need to develop additional physical means for effecting the ignition process for precision control and multifunctionality. Electromechanical excitation, which takes advantage of the underlying piezoelectric and flexoelectric behaviors of materials, is a prominent candidate mechanism. We report for the first-time a computational simulation framework that demonstrates that hotspot formation resulting from an internal dielectric breakdown is a previously under-explored mechanism for ignition.

The material considered here is an electroactive composite film comprising a copolymer matrix of P(VDF-TrFE) and embedded aluminum nanoparticles (~9% in volume fraction) subject to impact loading. To simulate the impact from a free-fall weight with variable drop-heights, a boundary velocity corresponding to the drop-height is prescribed. In addition, an electric field (*E*-field) is generated throughout the matrix, owing to its electromechanical properties. Both poled and unpoled P(VDF-TrFE)/nAl films are examined to assess the effect of poling. While piezoelectricity exists only in the poled films, flexoelectricity is present in both poled and unpoled films. To quantify the statistical variations in the behavior out of inherent material heterogeneities, a SEMSS (statistically equivalent microstructure sample set) with five random samples is generated and used.

Two successive analyses are performed. First, a fully-coupled mechanical-electrostatic analysis is carried out to establish the *E*-field induced by the piezoelectricity and flexoelectricity, leading up to the initiation of dielectric breakdown. Next, a coupled electrodynamic-thermal analysis is performed using the *E*-field obtained from the electrostatic simulation. Local temperature rise caused by resistive heating during the breakdown process and the local melting of the matrix are both accounted for, enabling us to accurately model the development of hotspots (i.e., critical regions characterized by localized high temperature) near the nAl particles. The hotspot field is used to establish the conditions for the onset of self-sustained chemical reactions in the film. The results show that piezoelectricity and flexoelectricity are essential mechanisms for charge accumulation that can ultimately lead to dielectric breakdown, hotspot development, and the initiation of exothermic reactions, with flexoelectricity having more significant contributions. Specifically, the poled films have ignition times ~10% shorter than those of the unpoled films. The findings are in good agreement with the accompanying experimental measurements.

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Simulating Nonlinear Domain Reorientation and Phase Transformation Phenomena in a Micromechanical Ferroelectric Model

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Key Words: *Ferroelectrics, Phase Transformation, Domain Reorientation, Power Supply.*

Ferroelectric generators (FEG) are often employed in pulsed power applications to deliver a short high-voltage and high-current pulse within a compact low maintenance design. FEGs deliver power by subjecting a ferroelectric element to a powerful mechanical shockwave that releases electrical bound charge by triggering nonlinear phenomena such as domain reorientation and phase transformation and less significantly piezoelectric response. Simulation challenges for FEGs arise from the difficulty in creating accurate nonlinear ferroelectric material models. Domain reorientation and phase transformations are difficult to model due to their anisotropic, nonlinear, and hysteretic behavior arising from irreversible changes in electric domain microstructure.

This work presents a micromechanical model that has been developed to accurately capture both domain reorientation and phase transformation phenomena in ferroelectrics. The micromechanical approach allows the approximation of the domain microstructure and nonlinear and an energy-based transition criteria is employed to govern changes in domain reorientation and phase transformation changes in the micromechanical framework. The ferroelectric micromechanical model is demonstrated for lead-zirconate-titanate (PZT) 95/5, a common ferroelectric material used in FEGs. PZT95/5 can be induced from ferroelectric to antiferroelectric phase through the application of compression due to a reduced unit volume in the antiferroelectric phase and in FEG applications display both domain reorientation and phase transformation behavior.

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A new paradigm to follow sharp physical interface - the eXtreme mesh deformation approach (X-MESH) - application to phase-change

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Key Words: mesh deformation, finite element, phase-change

The eXtreme MESH deformation approach is a new method to follow sharp interfaces without remeshing and without changing the mesh topology [1]. Moreover, the interface may change topology (nucleation, coalescence, splitting). The key idea is to allow elements to reach zero measure. This permits interface relaying, annihilation and seeding in a time continuous manner. The presentation will target the Stefan phase-change model in which the solidification front carries a temperature gradient discontinuity.

Traditional tracking approaches like the Arbitrary Lagrangian Eulerian (ALE) method are able to follow interfaces but cannot handle properly change of topologies of these interfaces. Other capturing approaches based on fixed meshes and enrichment strategies (as the extended/generalized finite element methods) may handle topological changes but at the cost of carrying extra degrees of freedom implying a special book-keeping and technical issues (as ensuring the time stability of the scheme with an evolving number of degrees of freedom).

The X-MESH keeps a fixed number of unknowns and a classical finite element approximation. The mesh deforms while keeping its topology. The nodes located on the solidification/melting front are not always the same because the front is relayed by the nodes. Examples demonstrating the capability of the X-MESH to handle nucleation and front coalescence will be shown during the presentation.

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Coupled simulation of vibration and sound radiation of Stradivari in large space

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Key Words: *Violin, Time evolution, Vibration, Acoustics, Numerical simulation*

The vibration and the sound field around the body of an old violin made by Stradivari are studied in this paper, where the highly precice geometry of the violin is scanned using a micro-CT scanner. After the noise in the scanned data is eliminated using a CAD software for post-processing, the geometry data are saved in the simulation software[1].
Assuming the orthotropic properties of woods (spruce and maple), the major vibration modes of the violin[2], such as A0, center bout rotation, B1-, B1+, and the acoustic pressure level at the surface of the violin body are calculated using the finite element method.
Next, using the sound pressure distribution at the surface of the instrument, the sound pressure spreading in a rectangular box simulating a concert hall is calculated with the open-source parallel acoustic analysis software: ADVENTURE Sound [3][4]. It is concluded that the sound pressure in the hall radiated from the violin is successfully simulated.

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Development of Partitioned Symmetric Formulation for Thermoelastic Interaction Problems

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Key Words: partitioned analysis, symmetric formulation, coupled thermoelastic problems, thermo-mechanical analysis, finite element method

This paper presents a partitioned symmetric formulation of transient coupled thermoelastic problems. The thermoelastic problem is multiphysics problem in which the wave (i.e. hyperbolic type) equation and the diffusion (i.e. parabolic type) equation are coupled. The classical formulation of thermoelastic problems is non-symmetric and has the paradox of infinite propagation speeds of thermal signals. As a result, the direct approach of this whole system is uneconomical, and special kinds of algorithms are required to solve the classical form. Based on this motivation, we introduce a partitioned symmetric formulation of thermoelastic problems. To do this, we construct two separate variational formulations of the uncoupled thermal conduction and uncoupled structural systems. These two uncoupled variational expressions are augmented by the constraint of energy exchanges between the elastic body and the thermal conduction body via the method of Lagrange multipliers. Finally, this paper suggests a solution algorithm including implicit-implicit time integration strategies, and the present partitioned formula is verified by one- and two-dimensional examples.

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Partitioned formulations for the simulation of dynamic Fluid-Structure Interaction problems using localized Lagrange multipliers

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Key Words: Localized Lagrange multipliers; Arbitrary Lagrangian-Eulerian; AFETI Partitioned Analysis

This work proposes a new Fluid-Structure Interaction computational framework for the solution of dynamic coupled problems. The coupling between the solid and an ALE incompressible fluid is formulated by means of the method of localized Lagrange multipliers (LLM) [1]. Instead of applying a direct coupling between the fluid and structure meshes, which is the traditional approach, LLM introduces an intermediate surface with its own degrees of freedom that is connected to the fluid and structure sides using independent fields of localized Lagrange multipliers. This approach facilitates the connection of non-matching meshes and allows us to derive explicit dynamic equations for the interface. The principal advantage of these dynamic interface equations is the uncoupling of the structure and ALE fluid problems, that now can be solved in parallel. Numerical experiments with the proposed methodology are used to prove its efficiency and accuracy by running a series of classical dynamic FSI benchmark problems.

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Simulation of interface-coupled porous-medium applications using partitioned methods

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Key Words: preCICE, partitioned coupling, porous medium, black-box methods

Many real-world applications involve porous-media multi-physics problems. Common applications are hydraulic simulations, where the hydromechanical coupling of a liquid in a fracture under high pressure and the resulting deformation of the surrounding porous medium is simulated, or the coupling of free and porous-medium flow, as it appears in simulations of water over a riverbed. In these cases, the problem can be split into two non-overlapping subdomains that are separated by a sharp interface. In each of these subdomains, the physical behavior and thus also the mathematical models to represent this behavior differ greatly. As a result, solving such a coupled problem using monolithic approaches leads to systems of equations that are ill-conditioned.

We present partitioned schemes that solve the problems on the subdomains individually in an iterative procedure. This allows us to reuse existing solvers for the resulting linear systems of equations while avoiding the assembly of the ill-conditioned monolithic system. The coupling of the subdomains is achieved by appropriate exchange of information over the sharp interface separating the subdomains and incorporating this information in coupling conditions. The iterative procedure is stabilized and accelerated by suitable interface quasi-Newton methods. Our focus is on black-box coupling methods that approximate the interface problem via information exchanged over the coupling interface. This black-box approach simplifies the reuse of existing software packages that are tailored to solve the individual subproblems. The couplings are carried out via the open-source coupling library preCICE [1] that has many useful features such as data mapping, data communication, parallelization, etc. already implemented. We study the behavior of different coupling schemes for hydromechanical coupled problems [3] and coupled free and porous-medium flow problems [2] to identify suitable coupling configurations.

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A high-efficient multi-scale analytical model of three-dimensional woven composites

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Key Words: *3D woven composites, Multi-scale analytical model, Strength prediction, Damage mechanics, Mechanical characterization*

Three-dimensional (3D) woven composites are being increasingly used in aerospace and automotive industries because of their better interlaminar fracture toughness, higher damage tolerance and improved mechanical stability [1]. To expedite their analysis and design efficiency, it is necessary to develop simple and accurate modeling tools capable of quickly evaluating their mechanical properties and progressive failure.

In this paper, a generic multi-scale analytical model for predicting stress-strain response and progressive failure behavior of 3D woven composites is presented. Firstly, based on apt geometrical approximation and assumptions, the unit cell (UC) of composite is firstly identified and reconstructed into a refined lamina structure with multiple equivalent lamina elements (ELEs). Micro-mechanical model (Chamis model [2]) is applied to estimate the elastic and strength properties of each ELE. Secondly, two-way coupled stress-strain responses between the UC (macro-scale) and ELE (meso-scale) are established through a bottom-up homogenization procedure and top-down localization procedure. Finally, a progressive damage model, which consists of damage initiation criteria (Hahisn-Hou failure criterion) and a stiffness evolution strategy (equivalent displacement method [3]), is employed to predict damage initiation and progression of the ELE.

The validated model is then used to evaluate the predictive capability of different unit cell model schemes and to investigate the effects of geometric parameters on stiffness and strength properties of 3D woven composites. The results indicate that the interior-surface integrated cell model scheme has the overall best performance in predicting mechanical properties of composites. In addition, an exponential model and a linear model are proposed to quantify the relationships between the number of weft layer and yarn density and mechanical properties, respectively. The present results demonstrate the analytical model can be a useful tool to provide an insight for the analysis and design of a range of 3D woven composites.

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Dynamic Analysis of Functionally Graded Graphene-reinforced Composite Sandwich Beams based on a Modified Zigzag Theory

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Key Words: *Modified zigzag theory*, *Sandwich beams*, *Free vibration*, *Natural frequency*, *Graphene reinforced composite*

With the extraordinary mechanical properties, graphene is regarded as one of the most attractive reinforcements for composite materials. However, for the natural frequencies prediction of functionally graded graphene reinforced composite (FG-GRC) sandwich beams, the current high-order models confront obstacles because of the ignorance of compatible conditions for interlaminar stresses. In this work, a modified zigzag beam theory is proposed for free vibration analysis of FG-GRC sandwich structures, which take into consideration the compatible conditions of transverse shear stresses at the interfaces of adjacent layers. Meanwhile, to enhance the accuracy of dynamic analysis, the Reissner's mixed variational theorem and preprocessing method of three-dimensional (3D) elasticity equations are adopted and implemented in the present method. The analytical solutions for such sandwich beams with simply supported conditions were provided by utilizing Hamilton's principle, and evaluated through comparing with 3D elasticity solutions as well as the results from existing high-order beam models. The numerical results demonstrate the precision of the proposed model in predicting natural frequencies of the sandwich beams. Subsequently, detailed investigation are carried out to explore the influences of the graphene volume fractions, distribution patterns, stacking sequences and other geometric parameters on the natural frequencies of FG-GRC sandwich beams.

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Local Refinement of Structural Kinematics for Failure Onset Analysis via Neural Networks

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Key Words: *CUF, Node Dependent Kinematics, Failure, Neural Networks, Composites*

The proper prediction of failure onset concerning load levels and spatial distributions is fundamental in the performance analysis of composites. A common approach is based on evaluating failure indexes obtained from combinations of stress components at any given point, and the resolution of the stress field affects the failure onset prediction. In composite structures, the complete 3D stress field – in-plane and transverse components – is necessary for many practical applications due to the anisotropic nature of the material. A typical example is the stress field around free edges where transverse shear and axial stress are dominating. However, proper numerical models to detect such fields tend to be cumbersome due to the necessity of using highly refined 3D meshes. An alternative approach is based on refined structural models to build 1D or 2D finite elements and relax aspect ratio constraints [1,2].
The use of Neural Networks (NN) in structural problems is increasing [3] due to their flexibility and ability in dealing with nonlinearities. This paper proposes a novel use of NN in combination with Node Dependent Kinematics structural models in which each node of the finite element discretization can assume a different structural theory. NDK is useful to augment the resolution of the model locally. NN is trained using different distributions of nodes to predict failure indexes. The output is the optimal refinement of the model concerning the structural model's order and where to use it. The use of the trained NN is helpful to localize the most critical areas to be modelled and set the proper structural model to use.

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Microscopic Stress Field Estimation of Unidirectional FRP having Random Fiber Arrangement under Transverse Tensile Loading by Image Analysis based Machine Learning

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Key Words: *Unidirectional FRP, Random Fiber Location Variation, Image-based Machine Learning, Microscopic Stress Field*

Composite materials are composed of multiple materials and are used in various fields because they have better material properties than single materials. However, random dispersion of the apparent material properties is larger than the case of the homogeneous materials, and a large dispersion of several properties such as apparent strength sometimes causes severe problems.

One of the reasons of this dispersion may be caused by random dispersion of a microscopic stress field in composites, but for example, even in case of a unidirectional fiber reinforced composite, it is difficult to predict the effect of random fiber location variation on microscopic stress state of the composite. A relationship between the arrangement of inclusions and stress state has been discussed in a few literature [1], but a general relationship in multi-inclusion problem seems to be unknown.

From this background, it is important to reveal influence of inclusions arrangement, in particular with considering randomness and uncertainty in the microscopic scale, on microscopic stress field and the apparent material strength. It is desirable to estimate the maximum stress and the location of its occurrence based on each fiber location, and the analyses with an image-analysis-based deep learning [2] or numerical information-based deep learning [3] were attempted. These reports suggested applicability of the machine learning for the analysis, but it was not clear whether a microscopic stress field was well learned or not.

From this fact, in this paper, applicability of the image-analysis-based machine learning to microscopic stress field estimation at each location in microstructure is investigated. Values of stresses at each location is learned, and accuracy and validity of the learning procedure are discussed with comparison of the previous learning results on maximum stresses and their occurrence location.

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Multiscale analysis of composite laminates

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Key Words: Composite laminates, Homogenization method, Computational continua

In practice, composite structures may exhibit more than two length scales. The O(1) homogenization method has been often employed in analyzing composite materials but had limited use for laminated structures. Since the composite plates or beams are often modeled as plane or one-dimensional structural elements (beam elements, shell elements and so on), periodicity in the existing multiscale analysis methods is mostly considered in the axial direction for beams and the in-plane directions for plates. This difficulty should be overcome based on an appropriate composite laminated theories.

O(1) homogenization method and computational continua (C^2) approach are employed to the multiscale analysis of composite beams and plates. Firstly, a two scale layerwise multiscale analysis method (LMAM) is established based on the RLWT and O(1) homogenization method for the composite laminated plates, considering the periodicity in in-plane and along the thickness direction simultanenously. And then, the two-scale and three-scale C^2 models of composite curved beams are developed; the four-node isoparametric beam elements based on the TSDT is employed to discretize the coarse-scale problems of composite curved beams, and the nonlocal quadrature scheme is employed to replace the classical Gauss quadrature since the size of Computational Unit Cell (CUC) is comparable to the size of the coarse-scale element. And then, a three-dimensional M^2 method is developed to analyze the local displacements and stresses in the woven composite laminate. The refined meshes in the every scale unit cells are regarded as the super elements, and their contributions on the macroscopic stiffness are smeared into the total stiffness matrix of macroscopic problem. The displacement continuity and internal force equilibrium at the interface between two different scale CUCs are ensured by a continuity equation set. At last, two-scale and three-scale C^2 models are extended into the composite laminated plates and woven plates based on the macroscopic TSDT and solid elements.

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Optimisation of multi-layered structures using a multispecies genetic algorithm and high-order structural models

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Key Words: *Optimisation, Multi-layered structures, Genetic Algorithm, Carrera Unified Formulation*

Due to the intrinsic nature of aerospace engineering, structural weight has always been an aspect of utmost importance during the design stages of aircraft and spacecraft. Indeed, light alloys were preferred for the construction of such structures until the irruption of composite materials. Currently, composite materials might represent more than 50% of the structural components of aircraft thanks to its mechanical properties and improvements in manufacturing techniques. In the recent years, fabrication procedures have been oriented to the additive manufacturing strategies, such as automated fibre placement or fused deposition modelling, which lead to multi-layered structures. As mentioned before, weight optimisation is one of the key steps in structural design. However, nowadays procedures, such as polar [1] or lamination [2] parameters, are based on assumptions that may shrink the design space. In this work, a direct optimisation genetic algorithm (GA) [3] is proposed. The presented GA is able to deal with discrete- and continuous-valued design variables, as well as including a multispecies capability, and new genetic operators. In this manner, several laminated structures can be considered at the same time in the optimisation loop in order to find the least-weight design that fulfils certain structural requirements. The latter are calculated by means of an in-house finite element code based on the well-known Carrera Unified Formulation (CUF) [4], in which high-order structural models can be obtained and used to analyse the mechanical performance of multi-layered structures.

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Stochastic microscale stresses prediction of variable angle tow plates considering multiscale defects employing unified finite elements and mechanics of structure genome

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Key Words: *Multiscale, Defect propagation, Variable angle tow, Carrera Unified Formulation, Mechanics of Structure Genome*

Advances in composite structures have permitted the conception of novel manufacturing techniques, such as Automated Fibre Placement (AFP) or Fused Deposition Modelling (FDM), that allow engineers to develop new families of laminated components. Indeed, thanks to these advances, variable angle tow (VAT) [1] laminates have increased their presence in aeronautic applications. Macro and mesoscale analyses of VAT structures has become available during the last decades, mainly focused on the buckling and post-buckling [2] behaviour. In the recent years, high-order finite elements, based on the Carrera Unified Formulation (CUF) [3] have been employed to analyse the free vibration [4] and stress prediction [5] of VAT plates and shells. Likewise, mesoscale failure onset [6] and buckling performance [7] affected by meso and microscale uncertainty defects has been addressed. However, due to the complexity inherent to the multiscale behaviour of composites, inner scales might have been disregarded when studying VAT composite components. In this manner, this work aims to analyse the microscale stresses that arise in the mentioned laminates subjected to uncertainty defects. For doing so, Mechanics of Structure Genome (MSG) is coupled with CUF [8] to provide: (i) homogenised material properties used in the macro/mesoscale analysis; (ii) retrieve the microscale stress state by providing the mesoscale strain state. Then, the latter can be utilised to calculate failure onset at the innermost scale of the structure.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Transverse Crack Characterization of Fiber-Reinforced Composites: High-fidelity and Data-Driven based Methods

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Key Words: Transverse Cracks, Machine Learning, Fiber-Reinforced Composites, Damage

Transverse cracks often are the first damage mechanisms starting in unidirectional plies of cross-ply fiber-reinforced composite laminates under multiaxial loading. Transverse cracks propagate towards the bounding plies and cause inter-ply delamination, which in turn reduces the structural integrity and undermines the mechanical performance. This work first integrates an efficient finite-element-based numerical framework with robust and accurate constitutive equations to study transverse behavior and multiple cracking of cross-ply fiber-reinforced composite laminates. The considered constitutive equations include elastic, elastoplastic damage, and cohesive zone models to simulate fibers, matrix, and fiber/matrix interfaces, respectively. The effect of fiber/matrix cohesive interface properties on the transverse crack density and delamination is investigated.

The developed high-fidelity framework is then used to generate a database to train a machine learning algorithm and predict the nonlinear stress distribution and failure pattern in microstructural representations of such composite materials. An image-based deep learning framework is developed. The deep learning framework contains two stacked fully-convolutional networks. A physics-informed loss function is also designed and incorporated to improve the performance of the proposed framework further and facilitate the validation process. It is shown that the proposed deep learning approach can predict the composites' post-failure full-field stress distribution and failure pattern, two of the most complex phenomena to simulate in computational solid mechanics, with an accuracy of 90%.

Data-driven Control of Bioaerosol Concentration by Inlet Air at a Recirculation Area Involved Indoor Corner

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Key Words: *Two-phase flow modelling, Machine learning, Recirculation area, Indoor air quality*

Indoor air quality attracts rich attention to the resident health, especially after the epidemic wreaks havoc all over the world. The air pollutants, such as virus, pollen, spores and fragments of fungi usually suspend and move with the indoor air as the form of bioaerosol. The recirculation area is found in an indoor corner, restricting the air-exchange with fresh air and providing a stable and comfortable for bioaerosol accumulation and growth. This research presents a novel concept to reduce the local bioaerosol concentration at indoor corner, via the actuated inlet air from ventilation outlet, through a data-driven controller design method. The feasibility of the proposed method is firstly analysed by a theoretical gas-particle flow model, in which the trajectory of a chaotic vortex is controlled to modulate the recirculation area by a data-driven orthogonal design scheme. The simulation results prove that inlet flowrate designed by a proper control signal reduce the local bioaerosol concentration successfully. Subsequently, the gas-particle laminar corner flow model is simulated by a commercial computational fluid software. The recirculation area at the corner is determined mathematically by the minimum net mass flux principle via grid search. A neural-network-based model predictive control is trained and designed to generate the control signal of inlet flow rate. The proposed control approach reduces 27.52% more bioaerosols than that without control interfere.

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Deformation-diffusion coupled material model for paper including visco-elasticity and visco-plasticity

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Key Words: Paper Mechanics, Paper Curl, Visco-plasticity, Diffusion, Finite Deformation

Paper is a material that is known for being sensitive to moisture changes, which renders its mechanical behaviour hard to predict. We propose a hygro-mechanical model for paper sheets that captures the transient behaviour during the paper's interaction with water. The proposed model provides insight into the interaction of mechanical dissipation phenomena in paper during liquid induced swelling. Such phenomena are relevant in industrial applications, e.g. for understanding paper deformation due to printing and packaging, as fluting and curl of paper depends on the generation of (dissipative) plastic strains [2].

The present work introduces a new model to the literature by employing a deformation-diffusion coupling in the logarithmic strain [3] and fluid concentration space [1]. We motivate a fully coupled theory since the diffusion of water within the paper network happens on a similar time scale as the mechanical relaxation phenomena. The switch to the logarithmic strain space is chosen as the incorporation of anisotropy can be performed in a straightforward manner and various mechanical effects (e.g. visco-elasticity and visco-plasticity) can be combined more easily. Besides, the absorbed water induces a large increase in volume which requires the application of finite strain theory. The model is derived in a thermodynamically consistent manner and its parameters are fitted to experiments available in the literature. The model yields a good agreement of numerical results with paper curl experiments and provides further insights into this complex multi-physics problem.

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Effect of High Mechanical Loading on Intervertebral Disc Calcification

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Key Words: *High Mechanical Load, Intervertebral Disc Calcification, Multiphysics, Charged Ions Transport*

High mechanical load (above physiological range) is related to spinal diseases such as intervertebral disc (IVD) degeneration and scoliosis, in which disc calcification has been observed. However, it is unclear whether high mechanical load is directly related to disc calcification. Thus, this study was aimed to investigate the effects of large mechanical load on the potential of IVD calcification inducement through anaylzing the intradiscal change of calcium (Ca^{2+}) and phosphate (Pi) concentrations under mechanical overload using a modeling approach.

A multiphysic mixture theory based finite element model of IVD was adopted [1] and extended to study the transport of Ca^{2+} and Pi in the negatively charged disc under three different levels of diurnal load, each consisting of an 8-hour rest at 100 N of compressive load and a 16-hour creep under compression at 500 N, 650 N, and 800 N, respectively. The disc was assumed to be in the electroneutrality state, the total charge of all ions (Na^+, Cl^-, c^F, Ca^{2+}, Pi) is zero,where c^F is the fixed charge density of the disc. In the disc, Pi exists in two forms, either dihydrogen phosphate ($H_2PO_4^-$), or mono-hydrogen phosphate (HPO_4^{2-}), the ratio of these two forms was determined by the Henderson-Hasselbalch equation. At pH of 7.2 in the disc, the valence of Pi is -1.5. The ultrafiltrable levels of Ca^{2+} (1.1 mM) and Pi (1.1 mM) in the serum were assigned as boundary conditions.

Concentrations of Ca^{2+} (denoted as [Ca^{2+}]) and Pi (denoted as [Pi]) in the IVD varied under diurnal mechanical load. In the nucleus pulposus, [Ca^{2+}] varied in the range of ~7-10 mM, [Pi] varied in the range of ~0.20-0.26 mM under normal diurnal load (100 N/500 N). Under large load, [Ca^{2+}] increased, but [Pi] decreased. The production of [Ca^{2+}] and [Pi] (denoted as Ca×Pi) was largest in the cartilaginous endplate (CEP) among all subregions of the IVD under all three loading conditions. The value was less than 2.4 mM^2 under normal diurnal load, but it was higher than 2.4 mM^2 under high load(i.e., 100 N/800 N).

Our simulated concentrations of Ca^{2+} and Pi were consistent with experimental data [2]. Mechanical load has significant effects on the spatial-temporal distribution of [Ca2+], [Pi], and Ca×Pi. Under high loads, our calculated value of Ca×Pi in the CEP reached the range (2.4-4.0 mM^2) for spontaneous precipitation of hydroxyapatite[3]. Our results indicate that high mechanical load may increase the potential of IVD calcification.

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Integrated features design and double optimisation of enhanced architected structural material for improved energy absorption

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ABSTRACT: Architected structural material is a class of materials integrating material properties and geometry, exhibiting new and highly customized behaviour that significantly filled up the empty spaces in Ashby plot as well as introduced new properties not available before. Based on published investigations and finding, the unique combination of structural design, enhancement and material constituent of these architected materials allow them to achieve extraordinary mechanical properties such as lower mass per unit volume, higher specific energy absorption per unit volume, high impact absorption, and more, compared with standard bulk materials. However, previously published work focused on investigating the effect of a single structural enhancement, such as hierarchy, graded, corrugated, etc**,** combined with cellular topologies, on the mechanical properties of the design. This work aims to develop a novel design principle, through both experimental and simulation investigation of the effect of combining of three or more structural enhancement into designs, and double optimisation with both conventional multi-objective algorithm and machine learning.

Key Words: a*rchitected material, design and optimization, energy absorption, machine learning*

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A Cohesive Traction Embedded Constitutive Law Combined with Tresca Yield Function and Shear-Induced Damage Variable for Ductile Failure

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Key Words: *DUCTILE FRACTURE, COHESIVE CRACK, TRESCA YIELD FUNCTION, DAMAGE MECHANICS*

The contribution of this study is to propose a cohesive traction embedded constitutive law [1] combined with Tresca yield function and shear-induced damage variable for a mixture with flat and shear-lip fractures in ductile failure. The two types of the fractures are represented by cohesive traction--separation law and shear-induced damage, since it is well known that these mechanisms are different from each other. For the flat fracture, the material stiffness reduction and strain softening due to void nucleation, growth, and coalescence under high stress state are realized by the cohesive traction separation law that determines the process of stress releases along with ductile crack opening. To realize crack nucleation at arbitrary location and propagation in an arbitrary direction, the cohesive separation law is combined with the Hencky-type hyperelastic-plastic model by the introduction of apparent strain due to crack opening and local balance equations between cohesive tractions and principal stresses. On the other hand, for the shear-lip fracture, the shrink of yield surface caused from the evolutions of voids in a shear band is presented by the shear-induced damage variable that is incorporated into the Tresca yield function. Moreover, the evolution of shear-induced damage is determined by the damage loading function corresponding to the plastic energy release based on thermodynamics [2]. Simple numerical examples are presented to demonstrate that the proposed constitutive law enables us to predict differences between flat and shear-lip fractures according to the thickness of specimens.

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A Crystal Plasticity Model for Porous HCP Crystals in Titanium Alloys under Multiaxial Loading Conditions

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Key Words: *Crystal Plasticity, Porosity, Porous RVE analysis, Homogenization; HCP crystals*

An efficient and effective crystal plasticity model is proposed for porous HCP crystals subject to a variety of multiaxial loading conditions. These conditions include (i) uniaxial, biaxial, and triaxial, (ii) tension and compression, (iii) low and high triaxiality, and (iv) axisymmetric and non-axisymmetric loadings. The framework is based on a combination of variational homogenization, phenomenological extensions, and assumptions motivated by observations from the high-fidelity micromechanical analysis. A novel penalty-free algorithm is employed to reach and maintain a specified stress state while performing representative volume element (RVE)-based crystal plasticity finite element (CPFE) analysis with porosity. The RVE studies demonstrate that the initial porosity, crystallographic orientation, and stress states have a significant effect on the homogenized mechanical responses of microscopically porous RVEs. The proposed porous crystal plasticity model is developed and calibrated using a database generated from the results of micromechanical RVE analysis. The calibrated porous model is reasonably effective in predicting the response of porous crystalline RVEs.

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A size dependent homogenized model for colonies of Ti-alloys having lath microstructure

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Key Words: *Crystal plasticity, Homogenization, Lath microstructure, Ti-alloys*

Near α and $\alpha + \beta$ Titanium alloys are widely used in aero-engine applications due to their excellent specific properties and thermal stability at moderately high temperatures. The microstructure of these alloys consists of equiaxed α grains having hexagonal closed packed structure and transformed colonies with alternate laths of α and β (body centred cubic structure) phases. The specific properties of these alloys can be optimized for a given application by modifying the volume fraction and sizes of these microstructural features; though such alloy designing solely using experiments can be expensive. Lately, Crystal Plasticity Finite Element Method (CPFEM) based analyses are being widely used to compliment the materials design process. However, a major challenge of using CPFEM based analyses for these alloys are the disparate length scales of the laths, and the colonies and equiaxed grains, in the same Representative Volume Element (RVE). In order to address this challenge, homogenized models of lath microstructure based on Taylor and virtual single crystal assumptions have been developed in the literature. However, these models fail to capture the traction balance at the interface on the homogenized response and hence lead to inaccuracies [1].

In the present work, an improved homogenized model has been developed that allows the interface to relax by undergoing a periodic motion while satisfying traction balance. Size dependency has been introduced by assigning anisotropic Hall-Petch based strengthening of slip systems depending on the Burgers Orientation Relation (BOR) between the α and β phases [1]. The homogenized model has been implemented as a user material subroutine pluggable into ABAQUS. The accuracy of the model has been evaluated by comparing its responses with CPFEM simulations of a single alternating α and β lath unit subjected to periodic boundary conditions following asymptotic expansion based homogenization. The other two existing models have also been considered in the comparative study. Two shear and two extensional deformation histories for two different Euler angles have been considered in the study. The comparison of the volume-averaged stress-strain responses showed that the model developed in this work is consistently more accurate than the other models. The phase stresses and slip activity in the developed model were also observed to be much closer to the corresponding volume-averaged responses obtained from the CPFEM simulations of single lath unit. The study clearly shows that the homogenized model developed in this work can be applied to perform CPFEM analysis of RVEs of near α and $\alpha + \beta$ Titanium alloys to predict both the macroscopic and local responses accurately. The model can also be applied to other material systems having a lath microstructure.

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Accelerated Multiscale Simulations of Heterogeneous Materials using Machine Learning with Knowledge Transfer

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Key Words: *Computational Homogenization, Machine Learning*

Engineering composite materials are largely heterogeneous in composition at the (macro) structural scale. In many complex applications, a predictive analysis of the structural performance is required. The grand challenge is to achieve a model with minimal constitutive assumptions and parameter calibrations at the macro-scale, while simultaneously retaining a similar level of predictive capability as direct numerical simulation (DNS) with full microstructural details, at a fraction of the computational cost required by the latter. One popular approach to achieve these competing objectives is to adopt a so-called FE-NN framework. At the micro scale, sampling points are generated by applying a macro deformation field to a representative volume element (RVE), over a wide deformation range, and extracting the corresponding homogenized response of the RVE. These sampling points thus form the database for the training of a homogenized surrogate model via Neural Network (NN), to be incorporated into a standard FE framework for analyses at the macro-scale.

The FE-NN framework has been shown to accelerate the structural analyses drastically, with predictions matching closely with DNS. One major limitation of the conventional FE-NN framework, however, is the huge database required for the training of surrogate model during the offline phase. In many applications, it was shown that the computational cost of setting up the surrogate model is comparing to a DNS, hence rendering it an impractical strategy for most applications. In this presentation, we focus on the computational cost during the offline phase of the FE-NN framework. Departing from the conventional approach, we first adopt a source model for the pre-training of surrogate model. The trained parameters are next downloaded for the training of the desired target model, to complete the offline training phase with knowledge transfer (KT). It is shown that the proposed KT-FE-NN framework reduces the computational cost greatly, compared to the conventional FE-NN approach. The predictive capability of the KT-FE-NN framework is demonstrated for several examples, benchmarked against DNS.

Advances in Practical Multiscaling

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Abstract

In my talk I will report on advances in developing a practical multiscale framework, including:

(i) A novel reduced order homogenization (ROH) approach based on nonuniform phase eigenstrain influence functions resulting in a response that is much closer to the first-order classical homogenization than existing ROH approach based on the uniform eigenstrain influence functions;

(ii) A pseudo-nonlocal fully integrated linear hexahedral macroscopic finite element based on reduced integration for stress updates but full integration for element matrices (residual and its consistent tangent stiffness);

(iii) A Bayesian Inference (BI) of the parameters of ROH where Neural-Network is first trained using the ROH, and then used as a surrogate model during the BI process; and

(iv) A coupled thermo-chemo-mechanical ROH for predicting residual stresses in fiber-reinforced polymer composites.

Atomistic-Continuum Multiscale Simulation of Polycarbonate Under Different Strain Rate Deformations

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Key Words: *Finite Element Method, Molecular Dinamics, Polycarbonate, Multiscale Simulation*

Polycarbonate is attracting attention as an engineering plastic with excellent impact resistance. In many applications, polycarbonate is used in environments where the stresses and impacts above the yield point are applied, such as external walls. Therefore, it is expected to analyze the behavior of polycarbonate before and after yield stress at different strain rates.

The yeilding is caused by the microvoids in the material[1]. However, It is difficult to trace the microvoids in the material at each strain by experiment. Molecular dynamics simulations at a large scale as in actual phenomenon take high analysis costs. Finite element simulations cannot represent the phenomenon of yielding due to microvoids. Therefore, the atom-continuum multiscale simulation is necessary to solve these problems in polycarbonate.

Kubo et al. developed a model for the coarsening of polycarbonate[2]. Urata et al. applied atomic-continuum multiscale simulations to amorphous solids[3]. Xu et al. measured stress-strain curves for polycarbonate at high strain rates (on the order of 10^3 s^{-1}) [4]. However, atomic-continuum multiscale simulations have not been performed on polycarbonate, a polymeric amorphous solid. Also, the behavior of microvoids at higher strain rates (the order of 10^5 s^{-1}~) is unclear.

In this study, molecular dynamics simulations are used to investigate the effect of increasing microvoids on yield stress. By applying the results to finite element simulations, the yielding of polycarbonate on the continuum scale is clarified from the viewpoint of the molecular scale.

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Coarse-Grained Atomistics at Finite Temperature by a Gaussian Phase Packet-Based Quasicontinuum

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Key Words: Multiscale Modeling, Quasicontinuum, Molecular Dynamics, Finite Temperature

Although being powerful simulation tools, atomistic techniques such as molecular dynamics (MD) come with severe restrictions: while only relatively small samples can be simulated, finite-temperature MD suffers from unrealistically high loading rates due to the time step limts of explicit time integration. Here, we discuss a finite-temperature quasicontinuum (QC) framework, which promises to overcome the aforementioned limitations by (i) spatially coarse-graining the atomistic ensemble based on a fully-nonlocal, energy-based QC approximation [1, 2] in an updated-Lagrangian setting, and (ii) using a statistical mechanics-based Gaussian Phase Packet (GPP) formulation for quasistatic finite-temperature calculations [3]. We show that the GPP ansatz includes the maximum-entropy QC formulation as a special case and captures local adiabatic heating due to atomic motion. Spatial coarse-graining limits full atomistic resolution to those regions of the simulation domain, where it is indeed warranted (e.g., in the vicinity of defects), while efficiently coarsening away from those regions. We discuss the fundamental concepts and the advantages and disadvantages of this simualtion framework, and we present a suite of example results, including dislocation interactions, grain boundary and surface properties of metallic materials as functions of temperature (comparing selected representative results to LAMMPS data for validation). Combined with automatic adaptivity, our simulation framework makes for a powerful toolbox for finite-temperature equilibrium and non-equilibrium simulations that overcome the length and time scale limitations of MD.

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Computational Homogenisation of Shear-deformable Shell Models accounting for Mesoscopic Damage in Laminated Composites

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Key Words: *Second-order homogenisation, cohesive elements, shear-deformable shell, laminate damage*

The progressive failure behaviour of large aerospace composite components is driven by damage phenomena that take place at the sub-millimetre length scale. The numerical analysis of these problems using full-scale high-fidelity modelling is often impractical, as the required computational resources increase exponentially with the structural size.

This work proposes a multi-scale framework that utilises shear-deformable shell and high-fidelity solid models at the structural and laminate length scales, respectively. The scale transition is handled using second-order computational homogenisation [1], where the mesoscopic damage events are described using the suite of progressive damage models developed at the Bristol Composites Institute (BCI) [2]. The downscaling constraints, consisting of a combination of surface and volume integrals, are derived based on a set of orthogonality conditions [3] with account for the cohesive interface elements at the fine scale. Due to the former consideration, both the curvature and transverse shear strains are accurately transferred from the shell to the solid models, showing no dependency on the RVE size for pristine (undamaged) laminates. During upscaling, the generalised shell constitutive laws are formulated in terms of the Taylor-bound and the fluctuation matrices [4], taking into account the stiffness contributions from the fine scale cohesive interface elements.

The proposed concurrent framework is implemented in the commercial finite element software Abaqus, where the nested FE^2 analysis is activated only for the shell material points in the critical regions. The framework performance is demonstrated through a series of comparative studies between full-scale and multi-scale models for flat and curved laminated composite panels.

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Computational Homogenization of Locally-Resonant Poroelastic Medium

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Key Words: Computational Homogenization, Reduced-Order Model, Poroelastic Materials

Currently, available soundproofing materials are crucial for mitigating noise in the automotive, aeronautical and building industries. They have remarkable performance at the mid- and high-audible frequencies. To obtain materials also applicable in the low-audible frequency range, it has recently been proposed in [1] to embed small particles within the material structure. As demonstrated in [1], the foam-like structure with a mass-spring effect creates bandgaps that can be tuned to target frequencies in the same fashion as locally resonant acoustic metamaterials (LRAMs). Wave propagation modeling in poroelastic materials poses computational challenges because of fine-scale processes at the pore level, for instance, air-solid drag forces, interacting with large-scale acoustic waves in the so-called subwavelength regime. In general, combining this intrinsically multiscale problem with finite-size geometries at the application (macroscopic) level becomes rapidly infeasible to solve due to limited computational resources. Multiscale reduced-order modeling arises as a promising approach mostly because it can preserve a high-fidelity model when a representative basis is selected, opening the opportunity to efficiently perform design optimization.

In this work, a transient computational homogenization framework is proposed for describing the dynamic macroscopic response of poroelastic materials with locally resonant components at the microscopic level. Extending the approach proposed in [2], the model is capable of capturing emerging exotic features such as bandgaps as well as the macroscopic Biot-like behavior of regular acoustic foams. Component Mode Synthesis is applied to reduce the fluid-structure microscopic problem based on a static-dynamic decomposition. Consequently, the formulation explicitly accounts for the contributions of the internal dynamics to the macroscopic physical quantities. Numerical examples demonstrate the efficiency and suitability of the proposed multiscale approach.

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Computational Homogenization of Martensite/Ferrite Interface Microstructures Towards Enhanced Cohesive Interfaces

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Key Words: Computational Homogenization, Dual-Phase Steel, Martensite/Ferrite interface, Substructure Boundary Sliding, Damage, Enhanced Cohesive Law

Martensite/ferrite (M/F) interface damage largely controls dual-phase (DP) steel failure. Several M/F interface models have been proposed in the literature, which however do not incorporate the relevant microphysics. Indeed, it has been recently suggested that the martensite substructure boundary sliding dominates the M/F interface damage and should be accounted for, placing a need of multi-scale frameworks. Moreover, depending on the activation of sliding, two distinctive M/F interface damage modes may occur: along the interface in case of inactive sliding; towards the ferrite matrix in case of active sliding, and both can lead to interface separation at the mesoscale. The sliding-induced interface damage mode nevertheless cannot be described with the existing multi-scale interface modelling frameworks. Therefore, a homogenization framework targeted for the M/F interfaces is developed. At the mesoscale, a DP steel mesostructure consisting of multiple martensite islands embedded in a ferrite matrix is modelled, with the M/F interfaces placed in between. The kinematics over the mesoscopic M/F interfacial zone entails a displacement discontinuity (and a deformation discontinuity) across the interface, which is internally enhanced by the sliding-induced kinematics. At the microscale, a M/F interfacial zone unit cell resolving the martensite substructure is considered. The martensite laths and inter-lath retained asutenite (RA) films are described using the crystal plasticity model. The ferrite matrix is described using a continuum damage model which incorporates the volumetric and deviatoric damage modes. Consistent with the mesoscopic interface description, two effective internal displacement jumps associated to the non-sliding- and sliding-induced interface damage modes, respectively, are defined from the correlated microfluctuations. Furthermore, applying the Hill-Mandel condition leads to the generalized interface tractions conjugated to these internal displacement jumps. Finally, an enhanced interface cohesive law is formulated, which accounts for two distinctive M/F interface damage modes. Numerical examples demonstrate the unit cell size-objectivity of the enhanced interface cohesive law obtained using the proposed homogenization methodology, and its power on modelling the M/F interfaces efficiently.

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Enhanced Non-Uniform Transformation Field Analysis

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Key Words: NTFA, multi-scale analysis, homogenization, reduced order modeling

We propose an extension of Non-Uniform Transformation Field Analysis (NTFA) [1] to address modeling of heterogeneous materials undergoing debonding. We denote the proposed method as Enhanced Non-uniform Transformation Field Analysis (ENTFA). Departing from the NTFA-based homogenization proposed in [2], we enhance it by introducing a consistent tangent matrix, and we formulate the enhanced approach for both single and multi-scale analyses. In the multi-scale setting, we adopt a suitable representative volume element of the micro-scale and model debonding with cohesive interfaces obeying the interface law in [3]. As in [2], the interfaces are partitioned into sub-interfaces, and the inelastic relative displacement field within each sub-interface is approximated by piecewise linear functions. This allows the inelastic relative displacements to be represented using reduced inelastic variables, which are solved for through a Newton-Raphson iterative approach based on the obtained consistent tangent matrix. This not only facilitates the derivation of the homogenized stress-strain constitutive relation at the macro-scale, but also allows to robustly trace complex snap-back phenomena in single-scale analyses by the application of an arc-length control technique. Several numerical tests demonstrate that ENTFA leads to a significant reduction of the computational time over reference non-linear finite element analyses, while retaining a satisfactory accuracy.

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Equlibrium shapes of homogenized prestrained composite plates

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Key Words: nonlinear plate, homogenization, prestrain, microstructure

The presence of prestrain has a tremendous effect on the mechanical behavior of slender structures leading to complex equilibrium shapes showing spontaneous bending, symmetry breaking, and wrinkling. We aim at predicting equilibrium shapes of microheterogeneous, prestrained, composite plates in the case of bending driven shape shifting. To this end we introduce a new approach that blends analytic and numerical methods. We start with a 3d nonlinear elasticity model for a periodic material that occupies a plate-like domain with small thickness. We consider a spatially periodic prestrain modelled via a multiplicative decomposition of the deformation gradient. By simultaneous dimension reduction and homogenization in the spirit of [1], we rigorously derive (in the Γ-limit of vanishing thickness and period) an effective, nonlinear bending model for plates with an emergent spontaneous curvature term in the plate model. The effective properties of the plate model (bending stiffness and spontaneous curvature) are characterized corrector problems. The general theory of Γ-convergence implies that minimizers of the effective plate model approximate minimizers of the original 3d problem, and thus, we study the dependence of equilibrium configurations of the derived plate model on properties of the 3d-composite. We do this exemplary for a parametrized sandwich plate with periodically distributed, prestrained fibres. To assemble the 2d-model, we first evaluate the homogenized properties of the 2d model by solving the corrector problems numerically (via standard Lagrange FEM). We then investigate the equilibrium shapes predicted by the 2d model. In the spatially homogeneous case, the problem reduces to an algebraic, non-convex minimization problem that can be easily solved numerically. In the general case, we appeal to a minimizing movement scheme to numerically approximate critical points of our plate model (this is a delicate task due to the presence of non-convex isometry constraint).

Our study reveals a rather complex dependence of the equilibrium shape on the considered parameters. E.g., the curvature and principal directions of the shape feature discontinuities in dependence of the volume fraction of the fibres; symmetry break: shapes may bend in directions that are neither parallel nor orthogonal to the fibre direction; size effects: strong dependence on the aspect ratio between the plate thickness and composite's period.

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Estimation of Nonlinear Material Behavior for Off-axis UD-CFRTP Using Numerical Material Tests

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Key Words:*UD-CFRTP, Numerical Material Tests, Nonlinear mechanical behaviour*

Unidirectional carbon fiber reinforced thermo-plastics (called "UD-CFRTP") not only possess anisotropic material responses, but also exhibit peculiar nonlinear material behavior depending on temperature and time [1]. The previous studies have suggested that such behavior could be characterized by performing numerical material tests (called "NMTs") with six macroscopic deformation modes (three vertical directions x, y, z and three shear directions xy, yz, zx) using the finite element (FE) model of a unit cell based on the homogenization method [2]. However, this setting is questionable especially when we examine the inelastic material behavior of UD-CFRTP under off-axis loading.

This study examines the anisotropic, nonlinear material behavior of UD-CFRTP under off-axis loading by conducting NMTs with more than six modes and proposes a method of identifying appropriate material properties of an assumed macroscopic anisotropic constitutive law. Specifically, seven macroscopic deformation modes (three vertical directions, three shear directions, and a deformation pattern in the off-axis direction of 45 degrees) are considered to prepare the virtual material responses to identify the macroscopic material properties by using an optimization method. To verify the identification accuracy, we compared the predicted macroscopic material responses with those obtained by the actual off-axis tensile test. In consequence, the extensive use of the NMTs technology with seven macroscopic deformation modes has enabled us to confirm that the material properties of the assumed macroscopic constitutive law for UD-CFRTP can properly be identified using the NMTs results with the off-axis macroscopic deformation mode in addition to the standard six ones in comparison with those using only six modes. It thus concluded that seven macroscopic deformation modes are indispensable for properly determine the nonlinear material behaviour for off-axis UD-CFRTP.

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Extended General Interfaces

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Key Words: Interphase, General interface, Interface elasticity, Cohesive interface, Interface position

Finite-thickness *interphases* between different constituents in heterogeneous materials are often replaced by a zero-thickness *interface* model. Well-established interface models intuitively assume that the interface layer is situated exactly in the middle of its associated interphase [1]. Furthermore, it is commonly accepted that this assumption is necessary to guarantee the balance of angular momentum on the interface. While the interface may coincide with the mid-layer of a uniform interphase, we argue that this assumption fails to sufficiently capture the behavior of graded or inhomogeneous interphases. We rigorously prove that the interface position does not necessarily have to coincide with the mid-layer in order to satisfy the angular momentum balance. This presentation introduces a novel interface model called extended general interface model which allows for arbitrary interface positions [2, 3]. The presented extended general interface model is essentially based upon the *weighted average operator* instead of the commonly *classical average operator*. Next, via incorporating this *extended general interface* model into homogenization, we develop bounds and estimates for the overall moduli of fiber-reinforced and particle-reinforced composites as functions of the interface position and properties. The significance of the interface position is demonstrated via a series of examples where the interface position is identified based on a full resolution interphase. Our presentation reveals several unfamiliar aspects of heterogeneous materials embedding interfaces and provides a deeper understanding of size-dependent behavior of materials [4, 5].

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Hierarchical Multiphysics Modelling of Fibre-Reinforced Composites

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Key Words: Multiscale Computational Homogenisation, Composites, Multiphysics Problems

The electrification of aircraft requires significant improvements to be made in thermal management, weight reduction, energy storage and electrical distribution. The use of multifunctional composites is essential in these endeavours and provides an effective way to significantly reduce the mass of components by using existing structural elements to perform additional functions. In fibre-reinforced composites, the mechanical and physical properties are highly anisotropic – with superior tensile strength, stiffness, thermal and electrical conductivities occurring in the fibre-direction rather than transverse and through-thickness directions. By tailoring the combination of fibre, resin system and nano-reinforcement used; these properties can be fundamentally optimised and significantly improved. However, the electrical and thermal behaviours of composites are poorly understood, particularly for complex geometries with different stacking sequences. The use of hierarchical, multi-physics modelling is essential to further this understanding to optimise both the micro-structural and macroscopic design of fibre-reinforced composites in a time-frame unachievable through manufacture and experimentation alone.

To understand this behaviour more thoroughly, a multi-physics, finite-element (FE) model has been produced to characterise the electrical and thermal conductivity of fibre-reinforced composites at the micro-scale. The 3D fibre architecture and resulting contact between adjacent fibres are responsible for the anisotropic conductivity. This fibre architecture has been reproduced using Bezier curves [1] to approximate fibre distributions from X-ray computed tomography data of 8552/IM7 composites [2]. A controlled degree of fibre overlap has been allowed, to form connections between adjacent fibres. The fibre architecture and its complementary matrix form a representative volume element (RVE). By applying periodic boundary conditions, an entire ply of material can be represented by a conductivity tensor given from Monte Carlo simulations of the micro-structure. Through rotational transformations of this tensor, a full laminate can be modelled using its stacking sequence. The model is capable of considering a variety of material combinations and ply stacking sequences to predict their electrical and thermal behaviour in a geometrically complex component. The detailed prediction of a composite's electrical and thermal behaviour is essential in developing the next generation of multifunctional materials.

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Kinetics of Ferroelectric Ceramics: A Large-Scale Phase-Field Study on Bulk Polycrystalline PZT

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Key Words: *Ferroelectrics, Domain pattern formation, Polycrystal, Finite temperature, PZT*

The thermo-electro-mechanical coupling and the unique property to permanently alter their atomic-level electric dipole moment (polarization) makes ferroelectric ceramics a promising active material for various engineering applications, e.g., in sensors, actuators, storage devices, energy converters, medical and communication industry. The complex coupling mechanism of ferroelectric materials requires multiscale modeling, reaching from the atomic level across the polycrystalline mesoscale to the macroscopic device level.

Based on a novel finite-temperature phase-field framework [1,2], which accounts for the temperature dependence of the DFT-informed Landau potential as well as thermal fluctuations, we perform high-resolution simulations of the ferroelectric domain evolution in a micron-sized polycrystal with an atomic-unit-cell spatial resolution by exploiting the parallel efficiency of the FFT-based numerical implementation. Results indicate that the switching kinetics of the effective material can be traced back to the evolution of the underlying domain pattern formation. The collective motion of domain walls, their interaction with grain boundaries, and the nucleation of new domains at the microscale result in a dependence of the homogenized material response at the macroscale on the loading rate of the applied electric field. Increasing the electric field rate at constant magnitude leads to a decrease of the remnant polarization, which agrees with measurements. Moreover, we observe realistic laminate-like structures within grains and show the impact of electric field rates on the domain pattern formation, which provides a deeper understanding of the emerging ferroelectric microstructure as well as its connection to piezo- and dielectric properties.

We present the development, realization, and validation of our finite-temperature phase-field framework and discuss its application to bulk polycrystalline (tetragonal) lead zirconate titanate and barium titanate to study the kinetics of ferroelectric ceramics, which demonstrates better predictions than competing models.

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Multi-scale Modelling of Emergent Dynamic Metamaterial Behaviour in Linear and Non-linear Regimes

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Key Words: Multi-scale Modelling, Computational Homogenization, Metamaterials, Wave Dispersion

Dynamic metamaterials exhibit emergent coarse scale wave dispersion behavior due to interactions between propagating mechanical waves and fine scale micro-inertia mechanisms, based on either localized resonance or Bragg scattering, or their combination. This opens new possibilities for advanced wave manipulation applications, e.g. tunable waveguides, adaptive passive vibration control, superdamping, acoustic diodes, cloaking and focusing, noise insulation and (vibro-acoustic) energy harvesting. The development and design of such materials and devices made thereof, requires advanced modelling techniques, capable, on one hand, to deal with complex geometries, boundary conditions and excitations, and, on the other hand, computationally more efficient than direct numerical simulations.

This talk will present a multi-scale technique towards efficient analysis of initial boundary value problems involving dynamic metamaterials of local resonance type in linear and non-linear regimes. The proposed approach originates from the classical computational homogenization, well established for quasi-static problems, an extension of which to transient problems has recently been developed. For linear problems, the static-dynamic decomposition can be used to derive the closed form homogenized equations representing an enriched effective continuum, in which additional kinematic degrees of freedom emerge to account for micro-inertia effects [1]. The application of this approach to metamaterials with negative effective mass, negative refraction index and attenuation of flexural vibrations of metamaterial beams and plates [2] will be illustrated. In non-linear case, fully coupled two-scale transient computational homogenization is used to study the wave dispersion in finite size macroscopic structures [3], demonstrating various phenomena emerging due to the presence of non-linearities, e.g. amplitude dependent attenuation response, higher-order harmonics generation and energy exchange.

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Nonlinear Multiscale Simulation of Beam Lattice Structures with Physics-Guided Artificial Neural Networks

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Key Words: Multiscale methods, Hyperelasticity, Convex neural networks, Metamaterials

Efficient multiscale simulation of finite deformations of soft composites and metamaterials requires the homogenization of effective constitutive models from microstructural simulations. Such effective material models must comply with continuum mechanical requirements, i.e., the laws of thermodynamics, material frame indifference, material symmetry, growth conditions, and ellipticity. While analytical models may not be flexible enough to capture the highly nonlinear behavior of soft microstructures such as beam lattices, data-driven models are more flexible, but so far they do not consider all requirements [1]. In this work, we present a data-driven constitutive modeling framework for the multiscale simulation of microstructured materials, which conforms to the physical model requirements by construction [2]. The strain energy function is formulated as an input-convex feed-forward neural network to fulfill the polyconvexity condition, which implies ellipticity. Two approaches are introduced: A model based on a set of polyconvex, anisotropic and objective invariants, and a highly flexible model that is formulated in terms of the deformation gradient, its cofactor and determinant. When calibrated with the challenging homogenization data of cubic beam lattices with instabilities, the invariant-based model shows drawbacks for several deformation modes. The model based on the deformation gradient alone is able to reproduce and predict the effective material behavior very well. Only a moderate amount of physically motivated calibration data is used, which shows the excellent generalization capabilities of these physics-guided data-driven constitutive models. Subsequently, the application in sequential multiscale simulations [3] and the extension towards parametric [4], inelastic and multi-physical materials are discussed.

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Numerical Material Testing for Compaction Process of Powdered Materials by means of FEM

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Key Words: *Powdered Materials, Homogenization, Multiscale, Compaction Process*

Powder materials are used in a wide range of applications including mechanical parts, pharmaceuticals and foodstuffs. The factors that affect the properties include not only the conditions related to the particles such as raw material, size distribution and surface treatment, but also the molding process such as granulation, filling, agitation, and milling. In particular, although compaction is an important process that determines the properties of the final product, there are few studies that have analysed numerically the material behavior in detail.

Material behavior of powders have been analytically predicted mainly by the discrete element method (DEM) [1]. However, DEM represents the rigidity of materials by adjusting the interaction forces between particles, so it is not possible to observe the deformation of individual particles. In this study, we conduct multiscale analysis of the compaction process by means of numerical material testing based on homogenization method [2] using finite element method (FEM) to predict mechanical behavior of powder materials. In order to create a microstructure model used for the analysis, we developed a Monte Carlo based algorithm which was confirmed that the filling rate close to the theoretical upper limit could be achieved in a very short time. We prepared two models having the particle size following uniform and Gaussian distribution. A numerical material tests were performed by defining the material properties for each particle as Elasto-plastic characteristic and macroscopic boundary conditions corresponding to the molding process. From macroscopic material responses obtained by averaging the results in microstructure, it was confirmed that the response depends strongly on the size distribution of the particles, and it can also be curve-fitted well by the Drucker Prager material constitutive law.

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Numerical Material Tests for Characterizing Macroscopic Viscoplasticity along with Static Recovery of Fiber-reinforced Thermoplastics

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Key Words: *Viscoplasticity, Kinematic Hardening, Static Recovery, Numerical Material Testing*

The static recovery is one of the relaxation terms associated with Armstrong-Frederick type kinematic hardening model and contributes to representing the rate-dependent mechanical behaviors of thermoplastic resin under non-monotonically loading[1], e.g., stress relaxation, strain recovery, and cyclic viscoplasticity. The present study examines the effect of the static recovery on the macroscopic rate-dependent mechanical behaviors of fiber-reinforced thermoplastics, comprised of thermoplastic resin and fiber material, using a method of numerical material testing[2]. The pure elasticity is applied to the fiber material for the sake of simplicity. On the other hand, the constitutive model of thermoplastic resin is adopted that of Launay et al.[3] which is slightly modified by considering the static recovery. Numerical material testing is conducted on the unit cell for unidirectional-reinforced thermoplastics after the constitutive model of thermoplastic resin is implemented to user-defined subroutine UMAT in the commercial software of finite element analysis ABAQUS. We discuss the obtained omni-directional macroscopic rate-dependent mechanical behaviors of fiber-reinforced thermoplastics and provide the guideline toward the establishment of a macroscopic constitutive model to realize a decoupled multiscale analysis.

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Realistic Microscale Domains through Microstructure Reconstruction

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Key Words: Microstructure reconstruction, Random heterogeneous media, Homogenization

A very relevant but comparatively little-researched aspect of multiscale simulations and homogenization is the generation of the microstructure geometry based on image data. While special cases like fiber composites have well-defined micro-scale geometries, many engineering materials are random heterogeneous media. For these complex materials, the exact micro-geometry is stochastic and unknown. While digitizing the full 3D geometry of a specimen through computed tomography or serial sectioning is often technically impossible or prohibitively expensive, obtaining microscopy images of one or few cross-sections can be much more feasible. In this contribution, differentiable microstructure characterization and reconstruction (DMCR) [1, 2] is presented, an algorithm that (1) efficiently constructs plausible 3D volume elements based on one or few 2D slices, (2) generates either one RVE or a set of SVE, and (3) can smoothly interpolate between different microstructures.

Unlike comparably efficient reconstruction algorithms, DMCR uses generic high-dimensional microstructure descriptors such as spatial n-point correlations. The advantages and disadvantages in comparison to faster and less general approaches in the literature are discussed as well as the range of applicability.

The novelty of this contribution is a rigorous validation of DMCR using real 3D data. For this, a single slice is extracted from the 3D data to mimic the case that only a 2D microscopy image is available. The reconstruction from this slice is compared to the original 3D data regarding the microstructure morphology and the homogenized properties. Using these two metrics, various parameters like the required number of cross-sections and their resolution are discussed in depth. Overall, this validation demonstrates the range of applicability of DMCR, allowing the homogenization community to assess its potential. This creates a basis for a plethora of possible future works that harness both microstructure reconstruction and numerical homogenization to advance scale-bridging simulations of complex materials.

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Surrogate model of computational homogenization for history dependent materials

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Key Words: *surrogate model, computational homogenization, history dependency, numerical material test, infinitesimal strain*

We propose a novel surrogate model for homogenized material behavior with history dependency. In recent years, data science techniques were introduced into the field of computational mechanics, and some kinds of surrogate models and data-driven methods have been developed to replace the classical constitutive model. In most recent, the history-dependent material behaviors represented by elastoplasticity have been paid exclusive attention as the target problem to be reproduced by the data scientific methods [1, 2]. Also, the applications of such methods for multi-scale problems have been studied in the interest of reduction of computational costs [3]. However, to the best of our knowledge, there has not been any surrogate model which can reproduce the homogenized stress-strain curves of composite materials with elastoplasticity including the unloading process. For that purpose, we developed a surrogate model which is capable to take the places of the macroscopic elastoplastic constitutive models within the infinitesimal strain theory. At first, to obtain the historical data of the macroscopic stress-strain relationships, we conduct numerical material tests on a representative volume element (RVE) by giving the various patterns of strain. Employing the macroscopic stress-strain history, we derive the histories of the macroscopic internal variables such as plastic strain and its accumulated quantity based on the computational homogenization theory. Arranging these historical data and performing some algebraic operations, we obtain a data set that represents the macroscopic constitutive relationship of the RVE. Using this data set, we construct a surrogate model by means of radial basis function interpolation with taking the step of the optimization of two hyperparameters. As the optimization method, we employ differential evolution, a well-known genetic algorithm. In the optimization process, we also perform cross-validation which saves the number of training data and ensures robustness in terms of variation of the input data for the surrogate model. In the presentation, we will conduct a surrogate computation of the load / unload problem of an elastoplastic material to verify the applicability of the proposed method for practical use.

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A Reduced Order Model Approach for Finite Element Analysis of Cellular Structures

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Key Words: *Lattice, Cellular, Finite Element, Multiscale*

Due to advances in modern manufacturing, there is an increased need for accurate and efficient simulation capability for microarchitected cellular structures. We define a cellular structure as a large macrostructure composed of individual cells, where the cells fit together to define the macrostructure. The cells need not be identical, the macrostucture may consist of a combination of solid material cells, plate-like cells, and truss-like cells. There exists a variety of asymptotic methods for simulation of cellular structures that are derived by assuming a separation of scales (infinitely small unit cells), with the detailed geometry of a unit cell replaced with a solid material with effective or apparent material properties [1]. The classic homogenization method, which assumes a periodic structure and uniform strain to compute the effective materials properties of the cell, is the most popular of these asymptotic methods. These asymptotic methods are quite efficient, but these approximations may not be accurate enough for critical applications. Conversely, the proposed Reduced Order Model (ROM) approach does not introduce effective or apparent material properties, but instead models the displacement of the unit cell by higher order polynomials. The proposed ROM is of intermediate complexity, it is more efficient (and less accurate) than a fully resolved finite element simulation, but more accurate (less efficient) than homogenization.

The proposed ROM begins with a highly resolved finite element mesh of a unit cell. A complete set of specially chosen high-order polynomial surface displacements is applied to the unit cell, and for each displacement the resulting force is stored. The resulting displacement-to-force map has units of stiffness, and after a change of variables this map can be used a drop-in replacement for a local high-order finite element stiffness matrix in a high-order finite element simulation of the macrostructure. The procedure is reminiscent of some FE2 methods [2][3], the key difference is that proposed ROM is based on high order polynomials. The overall approach is that a library of ROM's for different cells can be computed just once (offline phase), and used over and over again for difference macrostructures (online phase). In this presentation it is shown the proposed ROM converges to the full finite element solution as the order of the ROM is increased. In addition, the displacement and stress within the unit cell can be recovered.

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Elastocapillary and limited Plateau–Rayleigh instability of soft hydrogel fibers

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Key Words: surface tension, hydrogel, fiber, isogeometric finite elements, subcritical, instability

To date, the mechanics of interfaces of soft solids, e.g., polymeric gels, remain elusive. In particular, the mechanical properties of the bulk gel can differ from its boundary due to the fundamental role of surface tension and lower-dimensional energetics at length scales of nanometers to millimeters. From a theoretical perspective, classical continuum mechanics is size-independent and lacks a physical length scale. A characteristic length scale and size-dependent material response can be captured in continuum models by accounting for the energetic competition between the bulk gel and its boundary. This energetic competition, referred to as the elasto-capillary effect, plays a vital role in cavitation, soft composites, wetting on soft substrates, adhesive failure, and pattern formations such as beading, creasing, and wrinkling.

A fundamental challenge in understanding the behaviors of soft materials at small scales is the emergent instabilities due to complex elastocapillary stresses, e.g., the recently observed Plateau–Rayleigh (P–R) instability at soft gels. In *liquid* P–R instabilities, the surface tension overwhelms cylindrical columns and causes global undulations with a well-defined wavelength. However, the bulk elasticity will resist the capillary forces, playing a limiting role in *solid* P–R instabilities. The competition between capillary and bulk energies results in cylinders-on-a-string morphology in soft gels compared to spherical bead formations in liquid columns. This contribution aims to quantify the solid-surface competition and assess the highly nonlinear post-instability regime in soft solids at small scales.

The key focus of this presentation is to develop a computational framework modeling solid P–R instabilities using a surface-enhanced isogeometric finite element technique. First, we will show that the solid P-R instability is mainly a subcritical (discontinuous) bifurcation, which requires the development of path-following methods for gels to track stable and unstable equilibrium paths. Next, equipped with an arc-length-type nonlinear solution procedure, we study both the onset and the post-instability behaviors. We present numerical results illustrating the full evolution of P–R instability, observed in recent experiments with millimeter-scale hydrogel filaments. Our findings show that the soft cylinders form two distinct radii connected by a transition region with a finite width. Importantly, we show that the cylinders-on-string formations in hydrogels are highly tunable by controlling the applied stretch, residual stresses, and the characteristic length scale. The proposed methodology provides a robust computational foundation to elucidate elastocapillary instabilities in soft hydrogel fibers.

On wet coefficient of restitution of particles: a DNS study

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Key Words: *Coefficient of restitution, wet particles, DNS*

Global behaviour of wet granular flows is predominantly controlled by the exchange rates between particles and the carrier fluids at the microscopic levels. Therefore, accurate predictions of the macroscopic behaviour of the flow depend on the sub-models used to model the particle motions and their inner interactions. Among other parameters, the so-called "Coefficient of Restitution" (COR), defined as the ratio of the rebounding velocity to the impact velocity in a binary impact, is crucial as it directly impacts the nature of particle-particle interactions and the trajectory of particles in the flow, hence, the rates of mixing, and the energy dissipation in the system. While COR of dry impacts has been relatively well established, the problem of wet impacts and the effects of liquid bridging on the COR is still at the early stage of the investigations, see [1] and references therein. It appears that unlike a dry impact, which is essentially characterised by the impact force through mechanical properties of the particles and the impact velocity, a wet impact is far more complex, including cohesive [2], viscous and interfacial forces [3], and is currently an unknown function of the mechanical and surface properties of the particles, impact velocity, transport properties of the bridging liquid, intensity of the wetting, etc. [4].

In this paper, for the first time, we present fully resolved unsteady and multidimensional numerical simulations for wet impacts, using a new in-house DNS code that employs hybrid Levelset-VOF [4] combined with ghost-cell moving immersed boundary method. This enables fixed equidistance cartesian grids which in turn maximises the computational accuracy and maintains the CPU times at the minimum level. based on based on the. A series of simulations based on the experiments of Gollwitzer et al. [5] is carried out to computationally reproduce the wet COR of spherical glass particles impinging a wet planar surface. Time evolutions of the wave formations and liquid bridging are presented. The contributions of viscous and interfacial forces are calculated by calculating the time history of viscous dissipation and interfacial surface energies as a function of the thickness of the wetting liquid, diameters of the sphere and the impact velocity. COR for each case is calculated and compared with experimental data. Results are collectively discussed and the role of wetting on the COR is theorised.

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Design optimization of single phase metamaterial for elastic wave bandgap: graph theory and genetic algorithm based approach

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Abstract

Phononic metamaterials provide unconventional and unusual approaches to control the sub-wavelength elastic waves. In particular, locally resonant metamaterials (LRMs) attract great attention due to their potential applications as vibration isolation, low-frequency noise insulators, wave filtering, seismic wave mitigation, etc. It exhibits spectral gaps in the frequency range of two orders of magnitude lower than ones resulting from Bragg's scattering mechanism. Nevertheless, the formation of wide bandgaps in LRMs essentially requires the complex manipulation of multiple phases leading to difficulty in their fabrication. In order to overcome that problem, single-phase metamaterials with multiple bandgaps have been evolved in recent years. Although few attempts are made employing single-phase lattice structure to extract the wide bandgap; obtaining optimized configuration for the desired frequency bandgap through multiple parametric investigations is a challenging task. Therefore, the goal of the present study is to develop a numerical scheme for optimization of the single-phase lattice structure for desired frequency bandgap in the sonic range.

In this work, we provide a computationally efficient modification of the structure with predefined symmetry for tailorable bandgap. In particular, a graph theory-based approach will be used to represent the minimalistic unit of the lattice structure. Further, Analyzing the desired symmetric operations, the unit cells will be generated. Subsequently, connectedness upon boolean operation (addition and subtraction of edges) within the lattice is efficiently obtained. In order to achieve the optimized configuration GA based algorithm is performed. We adopt the beam element-based simulation framework for the extraction of dispersion response. Moreover, a more accurate evaluation of dispersion is obtained through the finite element procedure with the solid element. Consequently, we will also illustrate the mechanism of bandgap formation by addressing the local resonances with the vibration mode shapes. Then, the experimental investigation will be performed to validate the numerically calculated bandgap for optimized configuration. The present scheme will provide a numerical framework for the generation of optimized periodic units of single-phase metamaterials for the desired bandgap.

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Metamaterials parameter determination by means of an asymptotic homogenization applied in the finite element method

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Key Words: Metamaterials, Strain gradient theory, Finite element method, Homogenization

Different length-scales are fused together in additive manufacturing. For example a feature is called "infill ratio," where structure's weight is reduced by replacing the bulk with a periodic lattice substructure. A typical example is a grid or hexagonal infill, in this way, the weight but also the stiffness is reduced. Such a porous structure is technically a structure with a substructure that is known as metamaterial. We know that such metamaterials may be modeled by a generalized method. One possibility is strain gradient theory. In addition to the classical stiffness parameters, substructure related parameters emerge. Their determination is challenging.

The newly emerged parameters are substructure related. Hence, technically, by a given substructure, a homogenization method allows us to determine them. Based on asymptotic homogenization [1] a new formalism is applied in [2]. This procedure computes all effective material parameters in metamaterials by using a representative volume element incorporating the substructure. The computational procedure by means of finite element method (FEM) is developed with the aid of open-source packages. A brief explanation of the formalism, verification of the procedure, and examples will be given in this talk.

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Abnormal Grain Growth Induced by Nonuniform Grain Boundary Properties: Large-scale Phase-field Simulation vs. Mean-field Theory

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Key Words: *Abnormal grain growth, Grain boundary properties, Phase-field model, HPC*

Grain growth phenomena are ubiquitously encountered in the engineering of polycrystalline materials. In particular, abnormal grain growth, through which a few grains undergo preferential growth, is of great technological importance because it plays a decisive role in the development of high-performance materials including textured materials and single crystals. As a promising model for analytically describing abnormal grain growth, the mean-field theory proposed by Humphreys [1] is well known. Assuming that the abnormal growth of a particular grain is induced by its size advantage and the nonuniformity in grain boundary properties (energy and mobility), the mean-field theory enables the abnormal grain growth behaviors to be expressed as a function of only three parameters: the size ratio, boundary energy ratio, and mobility ratio between the particular grain and its surrounding matrix grains. However, the validity of this theory is not yet tested in detail, which is largely due to the difficulties in experiments for ideal model systems and the limited computational scales and accuracies employed in conventional simulation studies.
Our previous studies (e.g., Ref. [2]) have developed a large-scale simulation method for grain growth phenomena based on the phase-field modelling and parallel graphics-processing unit computing. In this study, we apply the developed method to abnormal grain growth and elucidate the validity of the mean-field theory via systematic two-dimensional and three-dimensional simulations on greatly enlarged scales with several hundreds of thousands of grains. The multi-phase-field model [3] is employed as the numerical model, enabling accurate treatment of polycrystalline grain boundary migration under the conditions of nonuniform grain boundary properties. A series of grain growth simulations are performed while varying the initial size ratio, boundary energy ratio, and mobility ratio of a particular grain and matrix grains. Detailed comparisons of the simulated results and theoretical predictions demonstrate that the abnormal grain growth behaviors (i.e., whether or not the abnormal growth occurs and the limiting size that can be reached by an abnormally growing grain) is well described by the mean-field theory.

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Analysis of Phase-Field Model for Solid-State Sintering

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Key Words: *Phase-Field Model, Solid-State Sintering, Thermodynamical Consistency, Free Energy Analysis*

Manufacturing materials by sintering for high-performance applications with tailored properties requires a deep understanding of the underlying microstructure evolution process. The Phase-Field method has been widely employed to model the microstructure evolution during the solid-state sintering process incorporating surface diffusion, grain boundary diffusion, and volume diffusion. An analysis of the well-known Phase-Field model in [1] is performed and shows that the free energy form employed in [1] may artificially introduce pores in solid grain boundaries where no pores exist initially, which is thermodynamically inconsistent. Additionally, the ratio of surface energy over grain boundary energy significantly affects this pore-generation artifact. Inspired by the work in [1, 2], a novel Phase-Field model is proposed to ensure thermodynamical consistency [3]. It is shown analytically and numerically that the artificial pore generation phenomenon is removed in the proposed model.

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Data Assimilation for Phase-Field Modelling and In-Situ EBSD Observation of Static Recrystallization in Aluminum Alloy

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Key Words: *Static recrystallization, Multi-phase-field method, Data assimilation*

The formability of aluminum alloys depends on their crystallographic textures. The textures are typically formed through static recrystallization that occurs during annealing. Hence, to produce aluminum alloys with superior formability, it is necessary to accurately predict static recrystallization and resultant texture formations. However, the mechanism of static recrystallization is still unclear and, therefore, intensive studies are widely undertaken to elucidate the recrystallization processes.

In experimentally observing static recrystallization, EBSD analysis is usually employed. However, it is difficult to reveal the whole picture of static recrystallization using EBSD analysis because it cannot observe the internal structures of metallic samples such as three-dimensional grain boundary configurations. Therefore, numerical simulation, which can analyse three-dimensional structures, is becoming common as a promising tool for the recrystallization study. In particular, the multi-phase-field (MPF) method is frequently used for simulating static recrystallization because the method allows for accurately reproducing polycrystalline microstructure evolutions. However, detailed data on the state variables and physical properties (e.g. stored energy) used in the MPF model is still not available due to the difficulty in their experimental measurement. On the other hand, data assimilation, which is a method for estimating unknown parameters in a numerical simulation by integrating observation data into the simulation, has attracted attentions as a means of improving simulation accuracy. It is expected that the accuracy of MPF recrystallization simulation can be improved by estimating the unknown parameter values via data assimilation. However, previous studies applying data assimilation to the MPF model [1,2] have focused only on simple curvature-driven grain growth, and the application to MPF recrystallization simulation is not yet attempted.

The purpose of this study is to estimate the state variables and physical properties such as stored energy by applying data assimilation to the MPF model of static recrystallization. Furthermore, we aim to elucidate the mechanism of static recrystallization by realizing highly accurate MPF recrystallization simulation. For this purpose, in-situ EBSD observation for static recrystallization of industrial pure aluminum was carried out to obtain observation data for data assimilation. We then estimated the state variables and physical properties included in the MPF recrystallization model by data assimilation using the in-situ observation results.

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Data Assimilation System for Dendritic Solidification with Melt Convection using the Phase-field Lattice Boltzmann Method

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Key Words: *Solidification, Convection, Dendrite, Phase-field Lattice Boltzmann Method, Data Assimilation*

Accurately predicting the formation process of solidification microstructures is critical for high-quality casting products. Recently, large-scale phase-field lattice Boltzmann simulations [1] and in-situ observations using time-resolved X-ray tomography [2] are performed to accurately elucidate the formation process of solidification microstructures. However, even such state-of-the-art technologies have major shortcomings, such as the lack of data on alloy material properties for simulations, and spatiotemporal resolution in observations.

Combining numerical simulations and experimental observations using data assimilation is a promising strategy for overcoming these drawbacks to enable highly accurate predictions of solidification microstructures. While data assimilation has been applied to elucidate some dendritic solidification processes, to the best of our knowledge, it has not yet been applied to dendritic solidification with melt convection.

In this study, we develop a data assimilation system using the phase-field lattice Boltzmann method [3] for predicting dendritic solidification with melt convection for the first time. The validity of the developed data assimilation system is confirmed through twin experiments for dendrite growth with forced convection, natural convection, and sedimentation of a solid grain.

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Data Assimilation using a 3D Phase-field Method for Dendrite Growth during Directional Solidification of a Binary Alloy

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Key Words: *Data Assimilation, Phase-field Method, Material Parameter Inference, Dendrite Growth, Directional Solidification*

Numerical simulations and experimental observations have made significant contributions to understanding the details of dendrite growth in alloy solidification. With the increase in recent computer speed, data science that enables integration of numerical simulations and experimental observations is attracting attention as the most promising approach. It is expected to overcome such conventional problems as low spatiotemporal resolution and limited information from experimental observations, as well as a lack of known material properties for the numerical simulations.

Yamanaka et al. [1, 2] first employed the data assimilation and phase-field method for the dendrite growth problem. Ohno et al. [3] proposed a method to infer interfacial properties of a pure alloy using data assimilation integrating molecular dynamics and phase-field simulations. In this study, we developed a data assimilation system combining three-dimensional (3D) simulations using the phase-field method [4] with time-resolved in situ 2D imaging using synchrotron radiation X-rays [5]. This was applied to dendrite growth during directional solidification of a binary alloy. Dendrites have a 3D structure, though the 2D imaging was conducted for a thin film sample. Thus, we performed an efficient 3D phase-field simulation using only the region immediately adjacent to the dendrite tip, as 3D simulations for the entire domain of the 2D imaging are challenging even now from the computational cost viewpoint. The developed data assimilation system was verified through numerical experiments, also referred to as twin experiments. Finally, we applied the data assimilation system to the 2D imaging of dendrite growth of an Fe-Si alloy.

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DMC-BO: Efficient Data Assimilation Method using Bayesian Optimization for Phase-field Simulation of Solid-state Sintering

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Key Words: *Phase-field method, Data assimilation, Bayesian optimization, Solid-state sintering*

Phase-field (PF) method is used for a powerful numerical simulation methodology to analyze microstructural evolutions during solid-state sintering. In order to quantitatively predict the microstructural evolutions by the PF simulations, accurate material parameters are required. However, many material parameters related to sintered materials, such as polycrystalline bulk superconducting materials, are unknown and immeasurable. On the other hand, cutting-edge experimental techniques (e.g., X-ray computed tomography) have realized the three-dimensional (3D) in-situ observation of microstructural evolution during the solid-state sintering [1, 2]. Therefore, recently, data assimilation (DA) has attracted attentions to estimate unknown material parameters from experimental data. DA has been developed for a computational technique that enables estimations of unobservable states and unknown material parameters by integrating time-series experimental data with the numerical simulation results based on Bayesian inference. In the previous study [3], particle shape, grain boundary distribution, and multiple material parameters were simultaneously estimated by applying the ensemble-based four-dimensional variational (En4DVar) DA method to a 3D PF simulation of solid-state sintering. Although En4DVar can estimate states and material parameters with high accuracy, it has a great challenge in computational cost. In order to overcome this challenge, in this study, we have developed a new DA method named DMC-BO [4]. DMC-BO uses Bayesian optimization (BO) to minimize the cost function which represents a misfit between simulation results and experimental data. DMC-BO is easy to implement in various simulation models because DMC-BO does not require the complicated calculations for deriving adjoint model [5]. Moreover, using BO reduces the computational cost for the minimization of the cost function. In order to validate DMC-BO, we conducted numerical experiments called twin experiments. The results demonstrate that DMC-BO is capable of simultaneously estimating the states and material parameters at less than half of the computational cost for En4DVar. Furthermore, the accuracy of the estimsted material parameters are reasonable for predicting the evolutions of the particle shape and grain boundary with high accuracy.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Investigating densification during sintering with phase-field and molecular dynamics simulations

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Key Words: phase-field, sintering, molecular dynamics

Sintering is an important process for many technical applications, but a full understanding still eludes the scientific community. Simulations are one key component of furthering this understanding by resolving the process from the atomistic to the mesoscopic process scale. Within the mesoscopic scale, the phase-field method has recently been used to simulate the sintering process by various authors. The employed models can vary drastically, even though the same process should be simulated, with no clear consensus on which model is the more correct one. In order to determine which models should be used and further developed, molecular dynamics simulations are employed to establish qualitative rules of motion during sintering. Following the determination of the rules, several published phase-field models and modified versions of these are tested for their compliance with these rules. Based on these results a phase-field model is developed for investigating the effects of sintering temperature and packing geometry in large-scale three-dimensional phase-field simulations. These simulations will be used to explain the enhanced densification observed in novel sintering techniques such as flash sintering.

Multi-phase-field Modeling and Simulation of Sintering

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Key Words: *Sintering, Mult-phase-field Method, GPU, Parallel Computing*

Sintered products are usually manufactured by filling powdered material into a mold, followed by the pressurization and heating of the material. Sintering is advantageous over casting in that complex-shaped products can be easily produced without melting the material. However, the products fabricated by sintering have lower strength than those fabricated by other working methods because the removal of pores is difficult. To address this issue and optimize the sintering process, systematic evaluations by a numerical simulation are indispensable. However, there are no well-established numerical methods to predict the microstructures formed during sintering with a high accuracy.

The phase-field method is the most powerful and accurate method for predicting the material structures at a meso scale. Wang [1] first applied the phase-field method to the sintering phenomena, based on which many sintering phase-field simulations have been carried out [2, 3]. However, it is difficult to accurately introduce surface/grain boundary properties, such as energy and mobility, as well as their anisotropy, into the model [1]. In addition, we need to reconsider the tensional force acting between two neighboring grains, which causes the rigid body motion.

In this study, we developed a sintering model based on the multi-phase-field model with a double-obstacle potential [4, 5], which can most accurately introduce the anisotropy of surface/grain boundary properties. Further, we developed a parallel computing code using multiple graphics processing units to accelerate the three-dimensional sintering simulations with numerous particles.

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Multiscale modeling and simulation of the crystallization, thermal sintering and thermo-mechanical response of semi-crystalline polymers

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Key Words: multiscale modeling, semi-crystalline polymers

An enhanced phase field model was developed for the numerical simulation of crystallization in semicrystalline polymers [1]. As with other models, it is based on coupling the heat equation with the Allen-Cahn equation, which is derived from the Gibbs-Thomson solid-liquid interface equation. Starting from the nucleation of spherulites, existing phase field models can simulate their evolution in a surrounding liquid and separate the amorphous and crystalline phases. However, the predictions of the morphological characteristics of the spherulites remain qualitative only. Moreover, the predicted spherulite evolution as a function of crystallization temperature is not consistent with experimental results. In our work, existing phase field models were enhanced in order to obtain experimentally consistent results. We target these characteristics to make them quantitative: spherulite growth, crystal morphology, and crystalline rate in spherulite. We show the importance of modeling the dependence of the model's parameters with respect to crystallization temperature, because, if assumed constants, the predicted results are not consistent with polymers physics. The model is numerically implemented using the finite difference method so that 2D and 3D simulation results are presented and compared to experimental data, illustrating the quantitative adequacy of the predictions with experimental evidence. Full-field micromechanical simulations were conducted on the microstructures generated by the enhanced phase field model in order to predict the effective mechanical properties [2]. A Fast Fourier Transform (FFT) method with periodic boundary conditions is used. Care is taken to obtain representative volume elements (RVEs) by computing the number of subcells in each spherulite and the number of spherulite nucleations in each RVE. Numerical FFT predictions of elastic properties for a range of crystallinity ratios are validated against experimental data and compared to simpler composite inclusion models. Finite element simulations of thermal shrinkage are also shown. We are currently extending the material description to a more realistic viscoelastic-viscoplastic model. The crystalline lamellae follow an orthotropic viscoplastic model based on the activation of slip systems, while the amorphous phase is (nonlinear) viscoelastic. Some properties can be identified directly while others are calibrated from reverse engineering. The procedure and its capabilities are illustrated for some polymers for which experimental data is available (e.g., stress-strain curves at different strain rates). A micromechanical model is currently being developed in order to predict the densification during a SLS (selected laser sintering) additive manufacturing process, and its impact on the mechanical response. All the models have been implemented in a research version of the Digimat software (from Hexagon Manufacturing Intelligence Division).

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Phase-field Simulation of Solute Segregation at Dislocation in Mg-based Alloys

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Key Words: *Phase-field Simulation, Solute Segregation, Dislocation Pinning, Mg-based Alloys*

To achieve wide applications of Mg-based alloys for structural components, extensive efforts have been made to increase the strength and formability of the alloys. It has been reported that an aging heat treatment of a pre-strained Mg-based alloy induces the solute segregation at dislocation, leading to the significant increase in the flow stress of the alloy (bake-hardening phenomenon) [1]. In this study, we performed phase-field simulations to obtain precise knowledge about the solute segregation behaviour and its effect on the pinning force of dislocation in Mg–Al–Ca–Zn system.

Elastic field of an edge dislocation was considered, and the solute diffusion driven by the inhomogeneity of elastic and chemical potentials in Mg–0.7Al–0.3Ca–0.3Zn (at.%) alloy was calculated by solving the Cahn–Hilliard equation. The simulation conditions of aging temperature and aging time were changed in the ranges of T = 413–473 K and t = 0–10^4 s, respectively. The simulated solute distribution was used to estimate the pinning force of dislocation; the dislocation was artificially displaced along the slip plane with fixing the solute distribution, and the elastic energy was calculated as a function of the dislocation displacement. The maximum gradient of the elastic energy–displacement curve was assumed as the pinning force of dislocation [2].

Segregation of Al, Ca and Zn near the dislocation core was observed in the phase-field simulation. Ca first segregated at the opposite side of the extra half plane, and subsequently, Zn and Al segregated at the side of the extra half plane. These results are reasonable in terms of the difference in the diffusion coefficients of solute atoms and the reduction of elastic energy derived from the dislocation and solute atoms. The segregation amount increased with increasing aging temperature and aging time, resulting in the increase in the pinning force of dislocation. Our simulation results show that the condition of aging heat treatment in a previous study (443 K, 1200 s) [1] is appropriate to achieve the bake-hardening effect derived from the solute segregation at dislocation.

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Phase-Field Simulation of Solute Segregation to Moving Grain Boundary in Multicomponent System

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Key Words: *Phase-field Simulation, Grain Boundary Segregation, Solute Drag, CALPHAD*

Overall properties of polycrystalline materials depend on the properties of individual crystal grains, distribution of crystallographic orientations (texture), and the properties of grain boundaries (GB). In various alloys, solute segregation to GB often occurs, leading to GB fracture and/or changing GB migration rate. Some theoretical models including phase-field models have been developed for predicting GB segregation [1,2]. However, past studies have mainly focused on the solute segregation to stationary/moving GB in binary systems, and there are few studies on the solute segregation to moving GB in multicomponent systems despite its practical importance.

In this study, the phase-field model for predicting solute segregation to moving GB in binary system developed by Cha *et al*. [2] was extended to the model for multicomponent systems. GB was treated as a distinguishable phase, and the Gibbs energy of liquid phase was substituted for the GB phase considering amorphous nature of GB. With a coordinate system that moves with GB, the movement of GB at a constant velocity was considered by adding a constant flux term to the diffusion equation of solute. Under this condition, one-dimensional steady-state profile of concentration and its drag effect on GB (solute-drag effect) was calculated. The Gibbs energy was directly extracted from existing CALPHAD databases using the Thermo-calc software [3].

As a case study, GB segregation and solute-drag effect in dilute magnesium alloys at 623 K were evaluated in Mg–Al–Zn, Mg–Zn–Ca and Mg–Al–Ca systems. The concentration profile around GB and the resultant solute-drag force were successfully obtained as a function of GB velocity. The simulation results show that the segregation behaviour in multicomponent systems is closely related not only to solute-solvent interaction but also to solute-solute interaction.

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Phase-field simulation of ternary alloy solidification in forced convection with local ensemble transform Kalman filter

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Key Words: *Solidification, Phase-field model, Computational fluid dynamics, Data assimilation*

The mechanical properties of alloys largely depend on their microstructures that are formed through solidification and subsequent metallurgical phenomena. Because the solidified microstructures in alloys are typically determined by the dendritic growth of crystals, it is necessary to accurately understand the dendrite growth for predicting the microstructural evolutions. Although direct experimental observations of growing dendrites have been reported in previous studies[1], it is difficult to measure the states of solidification such as solute concentration and flow velocity in a liquid phase from the experiments. Therefore, numerical simulations of dendrite growth using the phase-field method have been widely performed. However, many parameters involved in the phase-field models of alloy solidification are unknown. Our research group has proposed data assimilation methodologies to estimate the unknown parameters of the phase-field models from experimental data[2-6]. Specifically, the previous study[5] applied the local ensemble transform Kalman filter (LETKF), which is one of the most computationally effective methods for sequential data assimilation, to the phase-field simulations of alloy solidification. In this study, this LETKF-based phase-field model (LETKF-PF model) is coupled with the Navier-Stokes (NS) equation to account for the fluid flow in a liquid phase. Further, we perform numerical experiments to validate the estimation of the material parameters and the states including solute concentration and velocity fields in a Fe-C-Mn alloy. The numerical experiment results demonstrate that the present LETKF-QPF-NS model can simultaneously estimate the solute concentration field, velocity field, solute diffusion coefficient, and interfacial energy from the morphological data of a growing dendrite.

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Qualitative modeling of etch-pit formation (dissolution) on the K-feldspar surface through phase-field approach

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Key Words: K-Feldspar dissolution, Etch-pits, Phase-field method, Numerical simulation

Estimating the porosity and permeability of rocks is a necessary component of reservoir modeling. Feldspar dissolution is a widespread phenomenon in clastic bedrock reservoirs located in petroleum-bearing zones, affecting porosity, permeability, and thus reservoir quality [1]. We adopt a phase-field model to the dissolution of K-feldspar (Orthoclase) in the present work [2]. This leads in the formation and growth of etch pits, which vary in size and shape depending on the crystallographic orientation of the feldspar grains. We begin by calibrating the anisotropic model parameters to account for anisotropy in the surface energy and particle detachment kinetics at the feldspar-water interface. Calibration is accomplished by simulating the free growth of an etch pit in a single feldspar crystal and digitally replicating the formation and relative rates of the pits' different faces based on earlier experimental and numerical findings [3]. Following that, the calibrated model is used to simulate etch pitting in a variety of digital multi-grain packs with varied proportions of quartz and feldspar grains, analogous to sandstones. Furthermore, the digital grain packs are used to perform computational fluid dynamics analysis on the progressively pitted quartz-feldspar sandstones to determine their permeabilities. The proposed model is capable of recreating natural pit morphologies. The numerical data sets created are evaluated to determine the effect of etch pitting on the permeability, porosity, and mineral composition of sandstones, which is experimentally improbable or time consuming. Finally, we show the model's capabilities using novel post-processing and visualization techniques.

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The meso-failure of ceramsite lightweight aggregate concrete based on the phase-field model

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Key Words: *Lightweight concrete, Meso-failure, Phase-field, ABAQUS*

A phase-field model is developed to describe the meso-failure process of lightweight concrete containing expanded clay ceramsite aggregates. The phase-field model is applied to the meso-failure process of lightweight concrete by the ABAQUS subroutine user-defined element (UEL). The improved staggered iteration scheme with a one-pass procedure is used to alternately solve the coupling equations. In addition, the typical three-phase characteristics of lightweight concrete are incorporated into the phase-field model by generating mesostructures with mortar matrix, ceramsite aggregate, and interfacial transition zones through an automatic generation and placement program. The accuracy and effectiveness of the model in the cracking process of lightweight concrete meso-model are verified by the uniaxial tensile, three-point bending, and four-point bending common failures and mixed-mode failures of the meso-model of lightweight concrete are analyzed. The mesoscopic crack paths of the lightweight concrete calculated by the phase-field model are consistent with the transgranular fracture mode obtained by our test. At the same time, the crack appearance is similar to the results obtained by DIC, and the force-deflection curve is in good agreement with the experimental data in our test. The results show that the cracks of lightweight concrete specimens mainly occur in the ceramsite aggregates with weak strength, especially in the ceramsite aggregates with large particle sizes. The distribution of the ceramsite aggregates has a great influence on the peak load of the force-deflection curves, especially aggregates with large particle diameters. With the increase of the volume fraction of aggregate, the slope and peak load of the force-deflection curve decrease gradually, the bearing capacity of lightweight concrete specimens decreases, and the possibility of crack branching and coalescence decreases in the process of crack propagation. These examples show that the phase-field model can well capture the meso-failure process of lightweight concrete.

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Coupled QM/MM studies on Graphene deposited Silicon based photovoltaic solar cells in the presence of cracks

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Key Words: QM/MM, Graphene deposited Silicon solar cells, micro-cracks, multi-physics, electrical conductivity

Silicon is an abundant material on earth and is the primary choice in manufacturing photovoltaic solar cells. The fabrication of thin pristine Silicon solar cells involves several steps. As a result, defects like dislocations, micro-cracks and voids are unavoidable, and they tend to grow in the presence of multiple fields. Defects hinder the motion of charges. As a result, the charges will be accumulated around the defects [1, 2], which leads to the release of energy through recombination effects. On the other hand, the presence of defects alters the band gap in Silicon. Various authors studied the influence of mechanical and thermal loads on the band gap of Silicon [3, 4, 5] and reported that the band gap either changes or shifts from indirect to direct. The electrical conductivity improves when the bandgap decreases and vice-versa.

In this study, a multi-scale, multi-field analysis is performed using the QMMM package of Large-scale Atomic Molecular Massively Parallel Simulator (LAMMPS). The main objective is to study the performance characteristics of Graphene deposited Silicon solar cells in the presence of cracks. Initial cracks are created by deleting the bonds between the atoms on the crack surface. Furthermore, the cracks are opened by specifying a mechanical load in the form of tensile displacement, whereas, the thermal load is prescribed in terms of heat rate. During the entire simulation a quantum domain around the crack tip is considered to accurately estimate the electronic charge density of the atoms around the crack tip, and hence the electrical conductivity.

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A Novel Atomistic-Continuum Coupling Method for Amorphous Polymers at Finite Temperature

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Key Words: *Multiscale modelling, concurrent coupling, atomistic modelling, finite element method, amorphous materials, finite temperature*

In this work, a new simulation technique is presented for the concurrent mechanical coupling of particle and continuum domains at finite temperatures with potential application to fracture simulation in polymer nanocomposite materials. The coupling methodology is based on the Arlequin framework as proposed by Ben Dhia et al. for particle-continuum coupling in [1] and utilizes the concept of so-called anchor points for transmitting information between the two domains as developed in [2]. A bridging domain is defined wherein the particle and continuum domains overlap and forces and displacements may be transmitted. The present work draws upon the idea of grouping particles in the bridging domain to form Interface Volume Cells (IVC) as presented in [3]. These groups of atoms are then, in a spatially and temporarily averaged sense, connected by springs to respective anchor points in the continuum domain. This combination of techniques results in a new formulation that circumvents the need to connect continuum anchor points to individual particles, while benefitting from the inherent stability of a tunable spring-based load transfer mechanism.

In the present work, the particle domain is modelled using Molecular Dynamics (MD) in an all-atom representation at a temperature of 300 K and the continuum domain is modelled using the Finite Element Method (FEM). The two domains are solved iteratively until convergence is achieved for a given load state. Due to the continuum and particle domain time scales being vastly different, the FEM domain is solved statically, while the MD domain is run dynamically. A static uniaxial tension test is simulated using a three-dimensional block of EPON-862 resin, that is 85% crosslinked with curing agent DETDA. The applied loading is initially maintained within the linear elastic regime for model verification. Quantities such as stresses, Young's modulus, Poisson's ratio, and reaction forces are analyzed for convergence in the bridging domain and verified against a similar specimen modelled fully with FEM using experimental data available for EPON-862. After model verification in the linear elastic range, the loading is increased to simulate damage evolution and failure localization in the MD domain, in order to verify the post-yield behavior of the coupled model.

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Multiscale modeling of defect structures based on PN model

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A multiscale continuum model is developed to describe the defect structures in crystalline material such as FCC metals. The interface structure for twist, tilt and misfit grain boundaries are described by the dislocation network. The model incorporates both the anisotropy elasticity of each grain in crystalline materials and the molecular dynamics calculation informed interaction between two bulks, i.e., the nonlinear generalized stacking-fault energy. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twist, tilt and general grain boundaries. We also investigated the dislocation structure in heterogeneous crystalline material. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

Towards a robust multi-scale numerical modeling of the impact behavior of woven materials using equivalent microscopic fibers

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Key Words: *Finite elements, Dry woven fabrics, Ballistic impact, Multi-scale modelling, Equivalent fiber.*

A multi-scale modelling of the mechanical behavior of a dry 2D woven fabric subjected to a ballistic impact is developed in a combination between a mesoscopic description for the secondary yarns (not in direct contact with the projectile) and a microscopic description for the primary yarns (in direct contact with the projectile) in order to take into account the important fiber/fiber and fiber/projectile interactions in the impact zone. However, it should be noted that at the microscopic scale, a yarn is composed of approximately 400 fibers, the inclusion of which can significantly increase the computation time. For this, we have opted to introduce the notion of an "equivalent fiber" corresponding to 10 fibers. This proposed approach conducted to use 42 equivalent fibers in total to model a yarn. The effectiveness of this multi-scale strategy has been demonstrated by a comparison in terms of projectile velocity and projectile reactions, as well as degradation mechanisms of this multi-scale model with those obtained in the case of a complete mesoscopic modelling that were well validated with experimental data.

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A polarization-based multiplicative approach for modeling electrostrictive polymers

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Key Words: Finite strain electro-elasticity, electrostrictive material modeling, mixed finite elements

Electro-active polymers play an important role in today's engineering applications. Modeling and simulation of these materials, that respond to electrical stimuli by large-scale mechanical deformations, has been an active field of research during the last decade. Contrary to piezoelectric ceramics, that mostly operate in the linear range at a predefined polarization state, the electro-mechancial coupling in polymers is through higher order effects.

For the description of the deformation state, commonly displacement and deformation gradient are used. The electric field is the second independent quantity in many models. Thermodynamic potentials such as the free energy relate these independent fields to secondary fields: (total) stress and dielectric displacement. These secondary fields satisfy local equilbrium and Gauss' law. Different approaches for modeling electrostrictive behavior have been considered by various authors. A common approach is the prescription of field-dependent electric permittivities. An alternative is the introduction of a multiplicative splitting of the deformation gradient into an electric and a mechanic part, $\mathbf{F} = \mathbf{F}_{el}\mathbf{F}_{me}$ [1]. Multiplicative splittings are well-known from the modeling of visco-elastic electro-active polymers.

When such a multiplicative splitting is introduced to model electrostriction, the electric part of the deformation gradient is usually assumed as depending on the electric field, $\mathbf{F}_{el} = \mathbf{F}_{el}(\vec{e})$. However, in this case saturation of electrostrictive straining for higher electric fields that is observed in experiments [2] is not contained in the model. Therefore, we propose a different approach, where the electric part of the deformation gradient is considered depending on the electric polarization. In our models and also finite element implementations, we use dielectric displacement and polarization as primary unknowns, such that the electric field is seen as a secondary field. This way, by modeling saturation of the electric polarization, saturation of electric straining is a direct consequence. Additionally, Gauss' law of zero charges is satisfied exactly. A stable mixed finite element scheme for various element types is provided for (nearly) incompressible electrostrictive polymers.

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Modeling and numerical simulations of MEMS shutter devices

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Key Words: ADSR, MEMS, ALE, linearized flow equations

We investigate the acoustic behaviour of Micro-Electro-Mechanical-Systems (MEMS) with a focus on shutter devices. These shutter devices can be used for a new method of sound generation – which we call Advanced Digital Sound Reconstruction (ADSR) – where a redirection mechanism for sound pulses is incorporated [1]. With the help of this redirection mechanism, sound pulses can be generated which are superimposed to form an audio signal.
At MEMS-scales viscous effects can play a major role regarding sound transmission. Therefore, we utilize the linearized flow equations in time domain in order to solve for the acoustic pressure while incorporating effects caused by viscous boundary layers. Furthermore, the movement of the shutter itself contributes to the overall generated sound in a negative manner. Since the generation of the sound pulses is in the ultra sound range, the generated noise by the shutter might lead to adverse effects on the human body [2]. Hence, modeling the shutter noise and understanding its generation process can help to improve the design. To model the noise generated by the shutter, we apply the arbitrary Lagrangian-Eulerian (ALE) framework to the linearized flow equations to be able to compute the noise generation on the moving geometry. The geometry update itself is governed by an artificial quasi-static mechanical problem which is solved in each step to get the new element deformation [3].
Assuming that the impact of the acoustic pressure is negligible, a simple forward coupling from the quasi-static mesh-smoothing to the the linearized flow equations is employed. Furthermore, we use a direct coupling approach to couple the acoustic wave equation to the linearized flow equations. The final coupled system is then used to characterize the impact of the shutter movement on the overall system behaviour of a certain embodiment.

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Modeling viscous and thermal effects in acoustic actuators

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Key Words: Mechatronics, Multiphysics Problems, Acoustics, MEMS

Viscous and thermal effects are usually neglected when investigating acoustic phenomena. This is admissible if the corresponding boundary layer thickness remains small compared to the relevant problem dimensions. For air at standard atmospheric conditions the viscous boundary layer thickness is about 70 µm at a frequency of 1 kHz, which makes viscous effects relevant in important novel applications like micro perforated panels (MPPs) and acoustic actuators based on MEMS technology. A similar argument holds for the inclusion of thermal effects.

Several approaches exist to model viscous and thermal effects: Of course the flow field can be described by the full Navier Stokes equations, which need to be coupled to the flexible solid at the common interface. The resulting set of equations may be solved by, several numerical schemes, all of which share a large computational effort often rendering these methods unfeasible, e.g. for industrial applications. Another common approach is to linearise the compressible flow equations for small (acoustic) disturbances. Especially for cases without stationary background flow, this is often admissible, and the resulting equations can be solved employing the finite element method (FEM) [2]. Another approach is to employ an acoustic formulation in therms of the acoustic wave equation to model the flow field, and incorporate viscous and thermal effects in the boundary layers via an impedance type boundary condition [1]. This approach is computationally cheap, but is only applicable when the modeling assumptions of fully developed boundary layers are fulfilled.

Based on the example of a piezoelectric MEMS actuator, we demonstrate the importance of modeling viscous and thermal effects, with respect to the accuracy of the resulting acoustic field. We use a FEM formulation of the linearised compressible flow equations implemented in the open source finite element code openCFS [3]. We show how non-conforming interfaces can be used to couple solid and fluid domains without requiring conforming mesh at the interface. Finally, we investigate what assumptions in terms of mesh size, approximation order, and fluid domain size are suitable to minimize the numerical effort while maintaining acceptable accuracy.

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3D Modeling of asphalt materials at the mesoscale

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Key Words: *Asphalt, Mesoscale, Visco-elasto-plasticity, Creep*

To describe the mechanical behaviour of asphalts it is mandatory to numerically reproduce their internal structure, namely the location of bitumen and aggregates and voids. Subsequently, it is necessary to develop a sound mechanical prediction of creep, through a correct evaluation of the stress concentration among the inclusions and the voids within the domain of interest [1]. The mechanical behaviour at medium-to-long-term of asphalt is studied in the present work in a 3D mesoscale approach, by explicitly modelling the composite material as a cluster of aggregates (the coarse fraction is considered, for computational reasons) and bitumen surrounding them. The internal structure of an asphalt sample can be reproduced via a random disposition of inclusions, satisfying a given grading curve and a known volume fraction, as proposed in [2], when more sophisticated techniques are not available.
In agreement with recent viscoelastic formulations [3, 4] a novel visco-elasto-plastic constitutive model has been developed, where the viscoelasticity is accounted for via a fractional formulation, i.e. through a parabolic-dashpot-based mechanical representation. The subsequent non-integer order differential model is treated with the Grünwald definition of fractional derivatives. Long term effects have been carried out under different monotonic and cyclic load conditions, based on some relevant experimental tests. The model itself accounts for a better understanding of the inclusions interaction within asphalt under different compressive external loads.

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Three-dimensional visco-elasto-plasto-damage model for concrete in meso-scale

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Key Words: *Visco-elasto-plasticity, Damage, Cyclic loadings, Concrete*

A novel 3D comprehensive visco-elasto-plasto damage constitutive model of concrete is proposed to analyse the behaviour of concrete under long-term and cyclic loadings. This model combines the visco-elasticy and plasticity theories together with damage mechanics. The paper aims at providing an efficient model capable of predicting all the hysteretic characteristics of concrete material during cyclic loadings, taking into account time-dependent effects. The visco-elastic part is modeled within the framework of the linear visco-elasticity theory. The creep function is evaluated via the B3 model by Bažant and Baweja [1], and implemented with the exponential algorithm. The modified Menetrey-Willam [2, 3] pressure-dependent yield surface and a nonassociative flow rule are used for the plastic formulation of the model. The damage part of the model considers two exponential damage parameters, one in tension and one in compression, accounting for a realistic description of the transition from tensile to compressive failure [4]. The proposed model is calibrated and compared with uniaxial and multiaxial experimental tests.

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Fracture modelling of 3-D polycrystalline cathode particle embedded in a sulfide-based solid electrolyte for energy storage systems

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Key Words: *Solid state batteries; Polycrystalline Cathode; Interfacial Fracture; Bulk fracture; Phase field fracture; Diffused interface model*

All solid-state batteries (ASSBs) are promising candidates for "next-generation batteries" toward higher energy density, better thermal stability, and reduced flammability. The major obstacles for attaining the high energy density are the occurrence of chemical and mechanical degradations within the different components of ASSBs. In particular, the initiation and evolution of fracture within the grains, grain boundaries, electrolyte and electrode-electrolyte interfaces can cause capacity fade due to the loss of contact, reduction of material strength and transport properties under cyclic charge/discharge process. Stabilizing the ASSBs and extending their lifetime call for a high-fidelity electro-chemo-mechanical computational model that could be used for exploring the physical mechanisms and for identifying promising remedies through informed synthesis or operating conditions. In that context, a thermodynamically consistent multi-physics modelling framework is developed. In particular, it interprets the coupled electro-chemo-mechanical interactions in a battery cell, which includes the 3-D polycrystalline NMC cathode particle, sulfide based solid electrolyte phases, grain boundaries, and the electrode-electrolyte interfaces. For more realistic simulations, a secondary cathode particle is statistically reconstructed using the electron back scattering diffraction (EBSD) data and synthetic grain-architecture algorithm. In order to consider the initiation and propagation of crack within grains, grain boundaries, electrolyte and electrolyte-electrode interfaces, a regular phase-field fracture variable has been employed. A diffused phase field parameters have been adopted to define the transition of mechanical properties between the grains, grain boundaries, electrolyte, and electrolyte-electrode interfaces. Apart from incorporating the anisotropic material properties, the concentration dependent transport and mechanical properties have been considered. It is worth mentioning that the present model has been implemented in the open-source finite element (FE) package MOOSE for solving three state-variables: concentration, displacement, and phase-field damage parameter. Various parametric studies will be performed to explore the role of primary particle or grain sizes, secondary particle sizes, charge rates, interface properties and elastic modulus of the solid-electrolyte to correlate between the chemo-mechanical behavior and evolution of fracture on the electrochemical response of batteries. The present findings from the model offer predictive insights for designing the battery cell with reduced fracture evolution and enhanced electrochemical performance. Finally, the proposed model has been validated with the experimentally obtained characteristics of chemo-mechanical degradation.

Simulation of Piezoelectric Mechanism to Suppress Dendrite Growth

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Key Words: *Dendrite, Battery, Multiphysics, Modeling*

On immersing two lithium metal electrodes in a solution containing lithium salt and applying a voltage, lithium metal will deposit on the electrode connected to the lower voltage. This process is known as electrodeposition. It has been widely observed that under moderate currents, lithium ions do not deposit to a flat surface but rather spontaneously form sharp needle shapes known as dendrites. Dendrite formation is a major barrier for realizing the lithium metal battery, which not only causes capacity loss but also leads to internal short circuit and safety hazard [1].

We report a discovery that the use of a soft piezoelectric film as separator can effectively suppress the formation of lithium dendrite and stabilize the lithium surface during electrodeposition system [2, 3]. When the film is deformed by any local protrusion because of surface instability of the deposited lithium, a local piezoelectric overpotential is generated to suppress lithium deposition on the protrusion. We have established a theory that integrates electrochemistry, piezoelectricity and mechanics. We developed multiphysics computations to simulate dendrite growth in contact with a piezoelectric film. We find that the dendrite-suppression capability is over 6 orders stronger than the limit of mechanical blocking by any separators or solid-state electrolytes. Simulations show that the mechanism ensures deposition to form a flat surface even if the initial substrate surface has significant protrusions, suggesting its robustness and effectiveness against manufacturing defects. We show that the mechanism is so strong that even a weak piezoelectric material is highly effective, opening up a wide range of materials.

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A Moment-Accelerated Iterative Implicit Solver For The Multispecies 1D-2V Vlasov-Fokker-Planck– Ampére Kinetic Equation†

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Key Words: *multiscale preconditioner, VFP-Ampére, adaptive mesh, conservative discretization.*

We discuss a fully-implicit iterative solver for the Vlasov-Fokker-Planck—Ampère (VFPA) system with one configuration-space dimension and two velocity-space dimensions (1D-2V). The VFPA system couples a multispecies kinetic plasma description to the electrostatic electric field. The purpose of this work is to enable efficient, high fidelity, fully kinetic simulations of weakly- to moderately-coupled high-energy-density plasmas with an arbitrary number of species, particularly in regimes relevant to inertial confinement fusion (ICF). For many applications of interest (e.g., ICF implosions) the VFPA system exhibits large separation of numerical and physical scales in time and space, in particular due to the plasma frequency, fast electron motion, and electron collisions [1]. This numerical stiffness is addressed here by iterative implicit timestepping, accelerated by a high-order/low-order (HOLO) strategy (essentially a multiscale moment-based preconditioning scheme [2]). The scheme also employs an adaptive mesh strategy in physical and velocity space [3], in which the velocity space of each species is analytically rescaled and shifted by its spatially and temporally varying thermal speed and bulk flow, respectively; a moving mesh is used in the configuration space that allows tracking features with sharp spatial gradients, such as shocks and material interfaces. Further, conservation of mass, momentum, and energy, together with Gauss' law, are discretely preserved – commensurately with the iterative nonlinear relative tolerance – through a Lagrange-multiplier-like approach using nonlinear constraint functions [1, 4]. We demonstrate the effectiveness and accuracy of the algorithm with several benchmark problems of varying complexity, including a fully kinetic collisional plasma shock in planar geometry.

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A multiscale hybrid Monte-Carlo-Gaussian Coulomb-Collision Algorithm for Hybrid Kinetic-Fluid Simulations †

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Key Words: Monte Carlo, Gaussian, Coulomb Collisions, Particle-in-Cell

Coulomb collisions in particle simulations for weakly coupled plasmas are typically modeled by Monte-Carlo (MC) methods [1]. One of the main disadvantages of MC is the timestep accuracy constraint $\nu\Delta t \ll 1$ to resolve the collision frequency (ν) [2]. The constraint becomes extremely stringent for self-collisions in the presence of high-Z species, and for inter-species collisions with large mass disparities, rendering such simulations impractical. To overcome these difficulties, we explore a hybrid MC-Gaussian model for hybrid kinetic-fluid simulations. Specifically, we devise a collisional algorithm that leverages Maxwellians (i.e. isotropic Gaussians) [4] for both highly collisional kinetic species and fluid ones. We perform Gaussian-particle collisions using the Lemons method [3], which we have improved by more careful treatment of low-relative-speed particles. We extend the standard TA method for particle-particle collisions with arbitrary particle weights without losing conservation properties. The hybrid MC-Gaussian method is strictly conservative and is orders of magnitude faster than straight MC. We will illustrate the accuracy and performance of the proposed method with several examples of varying complexity, including relaxation and transport problems.

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Accelerating Radiation Transfer with the Variable Eddington Factor Method

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Key Words: radiation transport, kinetic effects, discontinuous Galerkin

The numerical simulation of radiative transfer is typically the dominant cost in the radiation-magneto-hydrodynamics codes used to model high energy density physics experiments such as the National Ignition Facility (NIF) at Lawrence Livermore National Lab. In fact, radiative transfer often accounts for 90% of the runtime and memory usage in simulations of NIF. This expense arises from the need for the accuracy of a kinetic model of the radiation field in these problems. A moment-based, reduced description of the kinetic equation allows the moment equations to couple directly to the other multiphysics components isolating the expensive inversion of the kinetic equation from stiff multiphysics.

The Variable Eddington Factor (VEF) method [1], also known as Quasidiffusion [2], is one such moment-based radiation transport algorithm. In VEF, the moment equations closed with nonlinear functionals computed from a discrete kinetic solution are iteratively coupled to the kinetic equation. Since these closures are weak functions of the solution, simple iterative schemes, such as fixed-point iteration, can converge rapidly. However, the low regularity of the closures and the unusual structure of the closed moment equations make leveraging existing discretization and linear solver technology difficult. Existing methods either rely on expensive and un-scalable preconditioners or leave solvers as future work. Without efficient solvers, VEF does not compete with traditional radiative transfer methods and is thus rarely used in practice.

In this talk, the unified analysis of Discontinuous Galerkin methods developed for elliptic problems presented in [3] is extended to the closed moment equations. The resulting VEF method is shown to have high-order accuracy in space, compatibility with high-order (curved) meshes, and efficient and scalable preconditioned iterative solvers. The method is tested on a challenging radiative transfer proxy problem and shown to scale to 1152 processors.

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Fast Evaluation of the Boltzmann Collision Operator Using Data Driven Reduced Order Models

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Key Words: Boltzmann Collision Operator, Reduced Order Models

With the emergence of novel applications of rarefied gas flows in hypersonic and space flights and microscopic flows, there is an increased need for simulation tools capable of handling complex flow geometries and of accurately predicting complex physics of the flows of non-continuum gas. The Boltzmann equation is believed to be the most accurate model of non-continuum gas. However, a major challenge continues to be the evaluation of the multifold integral describing the effect of molecular collisions.

We consider application of reduced order models (ROMs) to accelerating evaluation of the Boltzmann collision operator. To construct the ROM, a collection of solutions to the problem of spatially homogeneous relaxation of sums of two Gaussian densities are computed. Approximation spaces for the ROMs are formed by a subset of singular vectors of the solution data matrix [2]. Two cases of ROMs are considered. The first ROM results from a straightforward Galerkin discretization of the spatially homogeneous Boltzmann equation using a truncated basis of the singular vectors. The model approximates solutions to the Boltzmann equation accurately during early stages of relaxation. However, it suffers from presence of ROM residuals at later stages and exhibits polynomially growing modes for large ROM sizes. The second ROM evolves the difference between the solution and the steady state. The truncated singular vectors are orthogonalized to the steady state and modified locally to enforce zero density, momentum, and temperature moments. Exponential damping of ROM residuals is added to the model to enforce physical steady state solution. Solutions obtained by the second ROM are asymptotically stable in time and provide accurate approximations to solutions of the Boltzmann equation. Complexity for both models is $O(K^3)$ where K is the size of the ROM basis. For the considered class of problems, the models result in up to three orders of magnitude acceleration as compared to the $O(M^2)$ nodal discontinuous Galerkin (DG) discretization of [1], where M is the total number of velocity points.

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High-fidelity plasma simulations by coupling multi-species kinetic and multi-fluid models on decomposed domains with applications for Z pinches.

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Key Words: Multi-fluid plasma models, Continuum kinetic plasma models, Hybrid plasma modeling, Discontinuous Galerkin, Plasma sheath, Magnetized Kelvin-Helmholtz instability

A numerical method is developed for coupling a multi-species kinetic plasma model with a 5N-moment multi-fluid plasma model. The simulation domain is decomposed such that the local conditions satisfy the corresponding plasma model's region of validity. The method allows for hybrid simulations by formulating each model as a set of conservation laws and using a continuum numerical method to solve each model's governing equations in the subdomains of the decomposed domain. The models are coupled through fluxes across subdomain interfaces. Two methods are explored for the formulation of the fluxes that can be self-consistently represented by both plasma models. One method allows for flux calculations consistent with the 5N-moment multi-fluid plasma model and assumes thermodynamic equilibrium within each species of the kinetic plasma model. The second method ensures conservation of the distribution function as well as mass, momentum, and energy by formulating the fluxes using a composite underlying distribution function at the subdomain interfaces. The methods are compared in 1D1V simulations of a double rarefaction wave and a plasma sheath using the WARPXM framework, which solves each model using the discontinuous Galerkin finite element method. Both methods for formulating the fluxes perform well as the subdomain interface distribution function approaches a Maxwellian, with the consistent method being more robust to larger deviations. A simulation of the magnetized Kelvin-Helmholtz instability in 2D2V is also performed using the consistent method, which demonstrates the potential of the domain-decomposed hybrid method in facilitating speedup and reduction in required computational resources for high-fidelity plasma simulations, allowing for the investigation of problems that are beyond current capabilities. The coupling method is also used to study the lower hybrid drift instability, which is important to describing transport properties such as resistivity in Z-pinch plasmas.

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Low-rank Methods for Radiation Transport Calculations

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Key Words: Dynamical Low-rank Approximation; Radiative Transfer; High-order/low-order (HOLO)

The numerical solution of the radiation transport equation (RTE) is challenging due to the high computational costs and the large memory requirements caused by the high-dimensional phase space. Here we detail an attempt to reduce the memory required, and computational cost of solving RTE by applying the dynamical low-rank (DLR) method [1, 2], where a memory savings of about an order of magnitude without sacrificing accuracy is observed. The DLR approximation is an efficient technique to approximate the solution to time-dependent matrix differential equations. The desired approximation has three components similar to factors in singular value decomposition (SVD), and each of them is solved by integrating the matrix differential equation projected onto the tangent space of the low-rank manifold.

This talk presents our recent work that builds on the established DLR method and aims to enable low-rank schemes for practical radiation transport applications. We propose a high-order/low-order (HOLO) algorithm to overcome the conservation issues in the low-rank scheme by solving a low-order equation with closure terms computed via a high-order solution calculated using DLR [3]. With the properly chosen rank, the high-order solution well approximates the closure term, and the low-order solution can be used to correct the conservation bias in the DLR evolution. This improvement goes a long way to making the method robust enough for a variety of physics applications.

We also introduce a low-rank scheme with discrete ordinate discretization in angle (SN method) [4]. This low-rank-SN system allows for an efficient algorithm called "transport sweep," which is highly desirable in computation. The derived low-rank SN equations can be cast into a triangular form in the same way as standard iteration techniques.

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Moment extract method for solving kinetic dynamics of strongly magnetized plasma

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Key Words: *Fusion, Plasma, Kinetic dynamics, IMEX, Numerical scheme*

Collisionless dynamics of numerous numbers of charged particles, that is, *plasma*, provides common subjects and interests in studies of fusion, space, and astrophysical phenomena, where nonlinear evolution of the one-body distribution function of particles in the phase space needs to be solved together with fluctuations of the electromagnetic fields. In case with a background magnetic field, the charged particle motions are strongly anisotropic, and the field-aligned dynamics of electrons and electromagnetic fields govern the fastest time scales of the system after taking an average of the gyro-motion. However, in applications of fusion, space, and astrophysical plasmas, many interests are devoted to slower time scales than the parallel dynamics, such as the plasma turbulence and transport or fluid-like phenomena in a macro-scale. In other words, the fast parallel dynamics of electrons and electromagnetic fields are bottlenecks for an efficient time-integration of the plasma kinetic equation in a low-frequency regime.

In order to find a breakthrough in numerical schemes for the drift kinetic or gyrokinetic simulations of magnetized plasma, we have developed the moment extract method (MEM) [1] which decouples the zeroth and first order moment equations from the kinetic equation of electrons, preserving the full drift kinetic dynamics. The derived set of equations can be efficiently solved by means of an implicit-explicit (IMEX) scheme [2] when the phase speed of the electromagnetic (dispersive Alfven) wave exceeds the electron speed. The new scheme can relax the Courant limit for the drift kinetic simulation in the low plasma pressure limit.

In application to higher pressure plasma, where the electron speed may restrict the time-step size, we have applied the MEM to the semi-Lagrangian scheme developed for solving the Vlasov equation. The novel method demonstrates relaxation of the time step size both for the low and high plasma pressure cases, and improves numerical stability of the semi-Lagrangian scheme applied to the electromagnetic (Alfvenic) regime.

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Dynamic Local Coupling for Multiphase Flow: Balancing Efficiency and Stability

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Key Words: *Local coupling, Convergence stability, Operator splitting, Error Estimate, Multiphysics Problems*

Complex models involving numerous coupled physical processes create substantial computational challenge. This paper introduces a solver algorithm that maintains a locally fully coupled system in the subdomains in which individual physical process interacts with other processes strongly. Meanwhile, the solutions in the other regions are obtained in a decoupled fashion. The fully coupled regions are updated dynamically by either different timesteps or iterations.

Global coupling of multiple physics generally results in systems with large number of unknowns that are computationally unfeasible. In response, decoupling algorithms, such as three-way coupling of flow and geomechanics in porous media (Lu and Wheeler 2020), are introduced. Although alleviating the computational load, certain decoupling strategies commonly results in stability issues (Mikelić and Wheeler 2013), especially for nonlinear problems and sometimes encounters divergence during the solution process. The local coupling strategy applies error estimators to determine the strength of interaction between the physical processes in subdomains. By maintaining the system in fully coupled form within critical regions, the stability issue from the decoupling strategies is avoided while the computational load is significantly reduced as compared to a global coupling strategy.

The solver algorithm is tested with multiphase flow in porous media problem and provides up to 75% reduction is computation time. Additionally, such method could be applied to more complicated multiphysics problems such as fluid-driven fracture propagation (Lee, Wheeler and Wick 2016). Fully coupling of flow and mechanics in regions with crack propagation could facilitate the solution process. Previous method that decouples the two processes completely has caused significant increase in iterations.

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Multiscale model learning

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Key Words: Multiscale problems, multiscale methods, machine learning

We design novel multi-layer neural networks for multiscale simulations of flows taking into account the observed data and physical modeling concepts. Our approaches use deep learning concepts combined with local multiscale model reduction methodologies to predict flow dynamics. Using reduced-order model concepts is important for constructing robust deep learning architectures since the reduced-order models provide fewer degrees of freedom. Flow dynamics can be thought of as multi-layer networks. More precisely, the solution at the time instant n+1 depends on the solution at the time instant n and input parameters, such as permeability fields, forcing terms, and initial conditions. One can regard the solution as a multi-layer network, where each layer, in general, is a nonlinear forward map and the number of layers relates to the internal time steps. We will rely on rigorous model reduction concepts to define unknowns and connections for each layer. In each layer, our reduced-order models will provide a forward map, which will be modified (?trained?) using available data. It is critical to use reduced-order models for this purpose, which will identify the regions of influence and the appropriate number of variables. Because of the lack of available data, the training will be supplemented with computational data as needed. We will also use deep learning algorithms to train the elements of the reduced model discrete system. The work is partially supported by the Hong Kong RGC General Research Fund (Project numbers 14304719 and 14302620) and CUHK Faculty of Science Direct Grant 2020-21.

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A micromechanical approach for porous elasto-plastic hardening materials based on coupling full-field and mean-field homogenization methods

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Key Words: Porous plasticity, Modeling, Computational simulation, Homogenization

This work proposes an original and rather simple micromechanical approach to deal with the case of an elasto-plastic hardening matrix material containing circular or spherical cavities, in 2D and 3D respectively. The matrix can also be reinforced with solid particles. The purpose of the approach is to combine the high accuracy of full-field homogenization with the very low computational cost of mean-field homogenizatioon.

The strategy consists in coupling full-field (FE) homogenization for single cavity problems with Mori-Tanaka mean field homogenization at the representative volume element (RVE) level. First, a simple FE homogenization is conducted for a single cavity model (for both 2D and 3D cases) in order to get the homogenized stress-strain of an equivalent material called S. Then the actual porous RVE is alternatively modeled as being madee of solid spheres (or disks) of the actual matrix material embedded inside the material S. The volume fractions are determined from a maximum packing argument. Results were compared afterwards to reference simulations conducted on RVEs for 2D and 3D models. Very good agreement was found.

Next, for a particle-reinforced porous RVE (a three-phase material) the two-level strategy previously advocated for linear elastic materials by Naili et al.(2020) was extended to elasto-plasticity. Again, it was found that the proposed method exhibits very good accuracy.

The micromechanical strategy was successfully implemented and validated for the secant formulation of elasto-plasticity, which is restricted to monotonic and proportional lmoadings. Current work consists in extending the proposal to an incremental formulation of elasto-plasticity able to handle general loading histories.

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Clustering analysis for elastodynamic homogenization

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Key Words: Elastodynamic homogenization, Dispersion relation, Willis theory, Bloch waves, Clustering Analysis

This article presents a reduced-order method for the elastodynamic homogenization of periodic composites. With the help of Bloch-wave expansion and Green function, the Lippmann-Schwinger equations relating the dynamic field variable tensors of strain, velocity, stress and linear momentum are obtained. Then the constitutive relation of the averaged dynamic field tensors and the dispersion relation between frequency and wave vector in Willis theory are calculated directly. Using the data compression algorithm, k-means clustering, we decompose computational domain into clusters of possibly disjoint cells. The Lippmann-Schwinger equations are then discretized and solved efficiently. Numerical tests for 1D layered composites and 3D particle-reinforced composites verify the effectiveness and efficiency of the reduced-order method.

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Curvature induced size effect on the mechanical responses under indentation

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Keywords: *Curvature, Size effect, Nanoparticle, Molecular dynamics*

It is widely acknowledged that size effect on material properties exists at small scales. The influence of size on the strength of micro- and nanoparticles, which are the raw material for particle-based additive manufacturing technology, has drawn great attention but the universal conclusion still requires more efforts. Among all the methods, the nano-indentation carried out with molecular dynamics simulation is effective and attractive to investigate material properties and mechanisms.

In this presentation, nano-particles are examined with spherical indenters and we focus on the influences of particle size and indenter size simultaneously. All the simulations are run with Lammps code on the Explorer 100 high-performance platform of Tsinghua University. Particle radii and indenter radii covering a wide range ranges are examined to investigate their independent and joint influences. The ratio between the particle size and the indenter size is found to be an essential influential factor on the indentation curves, which categorizes the type of mechanical response of particles. When the ratio is fixed, the first yielding point increases monotonically with the size increasing, which implies that small particles may be easier to accommodate plastic deformation. Our results can be extended to more complex problems such as impact of micro particles on the substrate.

Data-driven Explicit Structural Topology Optimization with Hyperelastic Materials

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Key Words: *Data-driven, Topology Optimization, Finite Deformation, Hyperelastic*

Based on the constitutive theory, in the present work, a data-driven structural topology optimization method, which can solve the explicit topology optimization problem of the continuum structure with hyperelastic materials under finite deformation by only using uniaxial and biaxial experimental data, is developed. In this optimization problem, the aim is to minimize the compliance of the structure under the constraint of material volume. In addition, the degree of freedom removal technique is adopted to overcome the non-convergence problem of finite element analysis caused by weak material elements in the optimization process. Finally, some classic numerical examples are given to verify the effectiveness and stability of the proposed optimization algorithm.

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Data-driven Viscoelastic Material Model Based on Convolutional Neural Network and Prior Knowledge of Mechanics

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Key Words: *Material Law; Viscoelastic; Data-driven; Convolutional Neural Network*

In this work, a new data-driven method for building viscoelastic material law is proposed by combining characteristics of viscoelasticity theory and machine learning. Convolutional neural network (CNN) is used appropriately in this method to reduce the required amount of training data for machine learning. With only a small amount of data, the proposed method can learn the classical viscoelastic models described by a series of exponentials known as the Prony series. For a given displacement load, the trained model can predict the material response at the unknown moment. Results show that the present method can also predict the material law for complex microstructured materials with components described by another viscoelastic or elastic material models. Even under a complex cyclic loading, the accuracy of material behavior prediction can still be guaranteed. Limitation of the proposed approach is also discussed.

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FEM-Cluster based Analysis (FCA) and efficient prediction of the effective nonlinear properties of porous material

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Key Words: *Porous material, Cluster Minimum Complementary Energy, FEM-Cluster Based Analysis, Reconstruct the singular interaction matrix.*

The efficient prediction of nonlinear effective properties of heterogeneous materials is of great significance for their optimal utilization and material design. Based on the idea of data-driven clustering, Cheng et al. [1] proposed the FEM-Cluster based Analysis (FCA) to efficiently predict the nonlinear mechanical properties of various composite materials. FCA is different from the traditional computational micromechanics method which introduces reference materials and solves the discrete Lippmann-Schwinger (L-S) equation. In the FCA, the boundary value problem of the Representative Volume Element (RVE) is defined on a unit cell of the actual material and the interaction matrix can be regarded as the discrete Green operator, whose column vectors constitute the basis of the cluster self-equilibrium stress space. The step by step nonlinear properties prediction is carried out on the cluster-based reduced order model in the cluster self-equilibrium stress space by minimizing cluster complementary energy [2].
One of the recent developments of FCA is to apply the method for porous materials. We construct the reduced order model with no low modulus material filling in pores which was often seen in the methods such as the Fast Fourier Transform (FFT) to avoid numerical instability and convergence difficulties. It is interesting to discover the existence of the best low rank cluster self-equilibrium stress subspace, in which the projection of the interaction matrix reduces the cluster averaging errors and dimension of the reduced order model simultaneously. A reconstruction algorithm is proposed to define the best low rank cluster self-equilibrium stress subspace and construct the singular interaction matrix. Further, the unknown strain of the pore domain in the data-driven clustering reduced order method makes the Hill-Mandel inapplicable, the direct energy equivalence principle instead of the mean field theory is used to predict the effective properties of porous materials. Numerical examples are provided to illustrate the effectiveness and efficiency of this method [3]. Finally, the best low rank subspace and its related full stress vectors are being explored for the damage analysis of heterogeneous materials.

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Homogenization of steel-concrete interface in composite structures

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Key Words: steel-concrete interface, corrosion, composite structures, homogenization

Finite element analyses of reinforced concrete with the steel rebars can be particularly useful to evaluate the remaining life of aged structures accurately. However, the presence of ribs along the rebar length introduces geometric complexities which cannot be modelled explicitly for use in finite element analysis. To alleviate this drawback, a homogenized model of the interface consisting of rib geometry around the bar surface along with the concrete keys has been developed in this work. The asymptotic expansion homogenization method [1] is applied to evaluate the effective properties of the deformed bar-concrete interface. Owing to the axial periodicity of the rib geometry and concrete keys, the theory has been modified to incorporate the uni-directional two-scale response at the interface. An axially periodic Representative Volume Element (RVE) incorporating the geometric details of ribs along with concrete keys has been constructed. RVE analysis has been performed with appropriate strain boundary conditions applicable for a pullout test. A non-linear analysis has been used for capturing the equivalent maximum shear strength of the interface prior to failure. The results from RVE analysis has been used to obtain the equivalent homogenized stiffnesses of the interface and the maximum shear strength which have been further used in the cohesive zone model [2] which is based on Mohr-Coulomb material model. The developed homogenized interface model is validated from experimental pullout test results of deformed bars and would be further used to study the effect of corrosion on performance of structures.

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Investigation of Multiple Estimation Strategies of the Two-compartment Structure's External Thermal Load Identification using Neural Networks

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Key Words: *Thermal Load Identification, Multiple Estimation Strategies, Neural Network*

Identifying external thermal loads with limited measurement responses is important for the two-compartment structure, which is widely used in spacecrafts, when the real-time measurements of various loadings cannot be obtained directly. However, the measurement information from the limited number of sensors leads to an ill-posedness problem of inverse load identification. In this paper, A multiple estimation strategies based on neural network is considered, which narrows the solution domain of the problem step by step. The common issue of most of the literatures is the utilization of a single neural network to address this problem. In the multiple estimation, a combination of classification neural network and regression neural network has been proposed by author and it aims to gradually estimate the position and magnitude of thermal loads, respectively. A detailed description of multiple estimation strategies, neural network algorithm, data acquisition, and validation examples is presented, in order to show the effectiveness and feasibility of the proposed load identification method.

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Multiscale ANCF-FE^2 nonlinear analysis for composite material component

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Key Words: *Multibody dynamic simulation, Absolute nodal coordinate formulation, Finite element method, FE^2 method*

During the last few decades, flexible multibody dynamics has been widely used as an important theoretical basis. It has been frequently combined and used with the floating frame formulation (FFRF), which uses a local coordinate with an absolute coordinate. Within FFRF, the mass matrix will become nonlinear since the centrifugal force and Coriolis force are used due to the use of the local coordinate. On the other hand, the absolute nodal coordinate formulation (ANCF) has been developed recently to deal with the large deflection[1]. Within ANCF, the nodal coordinate of the element are described in the global inertial coordinate, so that the centrifugal force and Coriolis force may not appear but internal force may become significantly nonlinear.

Recently, investigation on ANCF related to biomechanics, space web, and soft machines has been actively conducted. Material characterization in the fields such as biomechanics, satellites and soft-machine machinery will require more sophisticated analysis to account for complexity of the relevant construction. However, further improvement in the constitutive relationship was required in the previous studies. Components used in those fields require use of the composite material, which are light and has improved strength and stiffness. Analysis upon the composite materials commonly requires multiscale modelling approach. And, a famous one of the multiscale modeling methods is finite element,[2] a versatile computational homogenization approach that is generally applicable for many material [2].

In this paper, multiscale modeling approach for a geometric nonlinear situation is suggested by using ANCF-FE^2 approach. This framework will connect micromechanics directly to existing ANCF element. Compared to the existing FE,[2] ANCF will obtain the exact Jacobian of the equation of motion in a straightforward fashion by using the invariance of the mass matrix and Jacobian simplicity of the constraint equation, [3]. It will be also straightforward to linearize the formulation which may exhibit advantage regarding the geometrically nonlinear analysis. Several numerical examples will be presented in order to demonstrate benefit of the present formulation.

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Multiscale analysis of composite plates based on Structural-Genome-Driven method

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Key Words: Data-driven multiscale method, Structural-Genome-Driven, Multi-level finite element method

In the design and fabrication fields of composite structures, multiscale problems attract considerable attention recently, such as how to obtain macroscopic constitutive models and track microscopic deformations simultaneously. Conventional multiscale modeling approaches, such as the concurrent homogenization methods, can deal with the problems, at the cost of the extremely high computational expense. In the data era, data-driven multiscale methods provide possibilities for solving the problems [1]. In this paper, an efficient data-driven multiscale method for composite plates is developed based on the Structural-Genome-Driven (SGD) method [2]. Firstly, the generalized strain and stress are adopted to construct the penalty function of data-driven framework of plate. Then, the multi-level finite element method (FE^2) is applied to collect the multiscale structural genome data for the database construction of the composite plate. Numerous offline microscopic calculations are performed within Representative Volume Elements (RVEs) using computational homogenization. Finally, the structural genome database is used to drive the online data-driven computing, whose results are compared with those obtained via conventional approaches to verify the accuracy and the efficiency. Since the conventional simulation process is decoupled into the offline data preparation and the online computing, in which the structural elements are employed for the simulations, the efficiency of the proposed data-driven approach is highly improved compared to the conventional one.

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Numerical Boundary Treatment for Shock Propagation in the Fractional KdV-Burgers Equation

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Key Words: Fractional KdV-Burgers equation, Shock wave, Boundary treatment, Machine learning, Ridge regression

We have proposed a numerical boundary treatment for simulating shock propagation in the fractional KdV-Burgers equation, based on a machine learning strategy. Numerical boundary treatment is particularly challenging due to the nonlinear and global interaction among the fractional diffusion, convection and dispersion. We select a suitable number of boundary points and interior points, and correct the numerical value at the boundary ones by linear combination of those at the interior ones. The large set of parameters are trained from a numerical reference shock solution connecting the end states 1 and 0, by ridge regression. Numerical tests demonstrate that the boundary treatment is effective in reflection suppression, and preserves the correct shock speed even under perturbed initial profile. Furthermore, using the above parameters, we construct a modified boundary treatment to simulate a range of different end states, with effectiveness checked numerically.

Numerical study of Gas Tungsten Arc Welding (GTAW) of a thin austenitic steel structure using two approaches: equivalent heat source approach and simplified approach

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The aims of this study concerns the simulation of GTAW in the field of multi-materials structure. The major topic concerns the thickness reduction of the stainless-steel sheets in the structure. In order to get an equivalent mechanical resistance compared to conventional ones, a composite material (fiber + resin) is applied by windings operation, with the objective to build a lighter structure. In this context, a program of tests and numerical simulations was defined, in order to predict, in a robust way, the final deformations due to welding operations. A comparison between experience and simulations, integrating the thermal and mechanical phenomena occurring during GTAW of stainless steels is performed.

The experimental part of this work was based on instrumented GTA welding tests. As far as the in-situ instrumentation is concerned, it was carried out on 1 mm thick metal sheet. Instrumentation was mainly based on thermal measurements by K-type thermocouples, displacements and strain measurements obtained by Digital Image Correlation technics, as well as arc welding current and voltage measurements.

In addition, cross-sectional macrographs of the weld seam were captured, in order to identify an equivalent heat source, for this process and in a butt weld configuration.

Thermomechanical simulation were then performed by using the equivalent heat source approach, taking into account the history of elements, namely the changes from solid to liquid and liquid to solid states. These simulations also take into account the real geometry of the beads due to addition of a filler material in the GTA process.

Using this approach, satisfactory results were obtained for thermal calculations. For mechanical calculations, determination of the bending angle of the sheets due to welding operation are also satisfactory, but calculations of the global displacements and strains of the sheets need to be improved.

A simplified approach was developed in parallel in order to reduce the CPU time. This approach is mainly based on the following observation: deformations generated by welding operations appear after manufacturing of the seams. According to our calculations means, this approach is the only one possible today, at the scale of a complete structure due to calculation time limitation purpose. Its implementation on simple sheets has just been carried out in this work: it allows in fine to reproduce the observed deformations obtained by DIC measurements without falling back on transient thermomechanical simulations, which demands too long calculation time, considering the scale of a complete assembly of structure. This approach is therefore quite promising.

On the coupling of Data-Driven computing and Model-Driven computing for composite materials and structures

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Key Words: *Data-Driven, Model-Driven, Coupling, Composites*

Multiscale simulation methods for composite materials and structures have been intensively developed during the past decades. The balance between the computational efficiency and accuracy remains one of the main issues. Recently, the Data-Driven Computational Mechanics [1] (DDCM) opens a new route to achieve this balance. By directly embedding the constitutive data into mechanical simulations, it bypasses the empirical material constitutive modelling, thus reduces the related cost and modelling error. Obviously, the development of DDCM could be accelerated based on the fruitful achievements of Model-Driven Computational Mechanics (MDCM, which refers to the standard constitutive model-based simulations), such as model reduction techniques, homogenization methods, domain decomposition techniques, etc.

In this work, we will discuss two potential combinations between DDCM and MDCM: (1) the data-driven computational homogenization method, where the multilevel finite element technique [2] (FE^2) is applied to construct accurate constitutive database, and the distance-minimizing data-driven approach is employed to reduce the online computing time; and (2) a domain decomposition coupling technique between DDCM and MDCM [3], where DDCM is employed for the local region to avoid material modelling errors and uncertainties, whilst MDCM is applied to the remaining regions to benefit from its computational efficiency.

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The Influence of Reinforcement-Matrix Interface Bonding on AMCs Effective Elastic Mechanical Properties - A Computational Study

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Key Words: *AMCs, Micro-Mechanics, RAE, RVE*

Aluminum matrix composites (AMC's) are composed of a ductile Aluminum matrix reinforced by stiff ceramic particles. AMC's, which are commonly manufactured using powder metallurgy, are highly attractive structural materials for the automobile and aerospace industries due to their high strength to weight ratio [1]. To improve the strength of the aluminum matrix, the use of ceramic particles composed of SiC, Al_2O_3, or B_4C is usually considered. TiB_2 is also a promising candidate for aluminum reinforcement. Nevertheless, while incorporating ceramic reinforcement to the aluminum matrix can result in increased yield and ultimate stress, it does not necessarily imply an increase in stiffness. The increase in AMC strength can be attributed to the localized stress fields among reinforcement particles, or the particles themselves acting as barriers for dislocation motion. On the other hand, the increase in stiffness depends on the load transfer between particles and matrix. The exact influence of the conditions of the particle-matrix interface on the effective elastic properties for such materials is still an open question.

In the present study a computational homogenization methodology is used to determine the effective elastic properties of AMC's by using both representative area elements (RAE) and representative volume elements (RVE). Simplified unit cell geometries were considered, as well as geometries constructed from micrographs. The first part of the study compared the effective elastic properties obtained for different particle volume fractions using RAE and RVE models. The second part focused on the influence of the particle-matrix interface conditions on the effective elastic properties in both tension and compression.

The study demonstrates that while RAE and RVE models produce similar estimations for the fully bonded condition, differences are obtained for the non-bonded case. It is also shown that increasing the volume fraction when the interface is weak reduces the effective elastic modulus and effective Poisson's ratio. The change in effective elastic properties is different in tension and compression, and can be correlated to differences in the mechanical interaction between the particles and the matrix. Compression experiments on Al-TiB_2 cylindrical specimens and ultrasonic testing for different particle volume fractions (0-15% TiB2) support the computational findings [2].

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Viscoelastic-viscoplastic polymer composites: development and evaluation of the two dissimilar mean field homogenization models

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Key Words: Micromechanics, Mean field Homogenization, Viscoelasticity-viscoplasticity

Materials are hierarchical in nature. Their macroscopic responses are strongly dependent to featured information at micro-scale. This multiscale nature of materials poses a continuing challenge in computational modeling of macroscopic structures.

This study proposes a micromechanical modeling of polymer composites with viscoelastic-viscoplastic (VE-VP) constituents. **Two mean field homogenization (MFH) models based on completely dissimilar theoretical approaches were developed within the infinitesimal strains framework** [1]. **The first approach is the incremental-secant method**. It relies on a fictitious unloading of the composite at the beginning of each time step. Then, a thermoelastic-like Linear Comparison Composite (LCC) is constructed from the computed residual state directly in the time domain. The method provides naturally isotropic per-phase incremental-secant operators for isotropic VE-VP constituents. It takes into account both the first and the second statistical moment estimates of the equivalent stress micro-field. **The second approach is the integral affine method**. It starts by linearizing the rates of viscoplastic (VP) strain and internal variables. The linearized constitutive equations are then recast in a hereditary integral format to which the Laplace-Carson (L-C) transform is applied. A thermoelastic-like LCC is built in the L-C domain, where MFH is carried out. Finally, the composite's response in the time domain is recovered by numerical inversions of L-C transforms. The method is able to overcome the issue of heterogeneous viscous stresses encountered by time domain MFH models.

The two proposed MFH formulations are able to handle non-monotonic, non-proportional and multi-axial loading histories. Their accuracy was assessed against full-field finite element (FE) results for different microstructures and loadings. **The computational cost of both methods is negligible compared to FE analyses**. Overall, **the incremental-secant approach is much simpler mathematically and numerically than the integral affine formulation, its accuracy ranges from acceptable to excellent**, and important improvements can be expected in the future by controlling the virtual unloading time increment.

Currently, the incremental secant model is being extended to the finite strain framework. The objective is to further consider strain softening and re-hardening of constitutive materials at large VP deformations.

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A physics-constrained deep learning based approach for 2D acoustic metamaterial design

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Key Words: *Material Design, Inverse Problems, Acoustic Wave Scattering, Machine Learning, Deep Auto-encoder*

The control of acoustic and elastic waves through metamaterial design has been an interesting subject with great potentials of various applications such as non-destructive evaluation of structural, biomedical devices [1], high-resolution imaging, radar and remote sensing. To date, there is still a lack of powerful and efficient design methodologies since the conventional optimization-based approaches suffer from the computation burdens in parameter search whenever a design query is made. In this study, a deep auto-encoder (DAE) [2] based approach is proposed to design the geometry of wave scatterers that satisfy the user-defined downstream pressure fields. The estimation of scatterer geometry is strengthened with the latent representations of the pressure fields learned by the DAE. Once the training is finished, given a target 2D pressure fields, the proposed approach achieves an accuracy of 99.91% on the testing data, and the inference efficiency is enhanced by a factor of 195, compared to the baseline reference implemented using the genetic algorithm. Furthermore, the generalization capability of the proposed network is validated through a dataset generated with new shapes of wave scatterers. Lastly, this study provides an insight into the interpretation of the convolution layers in the network [3]. Numerical simulations and design examples are presented to demonstrate the robustness of the proposed approach.

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Elastic Metasurface and Its Applications

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Key Words: *Metasurface, Elastic Wave, Generalized Snell's Law*

Elastic metamaterials, which have been an active research area in the last two decades, come from improving the high working frequencies of periodic structures. The frequencies which make the left-handed metamaterials casue the refracted waves to bend into a negative direction. Metasurface, which is a thin layer in subwavelength scale, manipulates waves through phase shifts. Instead of three-dimensional left-handed metamaterials, metasurfaces use simple planar designs to produce the same effect. The planar fabrication process is cost-effective in comparison to the manufacturing of the complex 3D metamaterials. Since Yu et al. [1] designed the V-antennas to demonstrate generalized Snell's Law, metasurfaces have been studied extensively. This study focuses on elastic waves. Through different elastic metasurface designs, anomoulus refractions and corresponding applications are achieved.

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Evaluating Bistsbility of Phase Transforming Cellular Materials with Finite Element Analysis

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Key Words: *Material Design, Metamaterial, Bistability, Finite Element Method*

Metamaterials exhibit supernatural properties which cannot be realized with bulk materials owing to their periodic structures in order of nano-, micro-, or milli-meter. Lately, additive manufacturing (AM) technologies have been applied to the fabrication of metamaterials with cellular lattice structures which are specially designed unit cells exhibiting novel mechanical properties such as auxetic materials having negative Poisson's ratio. Recently, bistable metamaterials that can convert their geometry reversibly between two or more different stable or metastable configurations have been researched. From the similarity of the geometric transformation of these bistable metamaterials and phase transformation of crystalline materials, these metamaterials are called phase transformation cellular materials (PXCM) [1]. In our previous research, for the purpose of investigating the relationship between the geometric design and bistable property, we conducted a compression test for PXCMs in various geometry [2]. In the present study, for analysing the criteria for the phase transformation, the deformations of the bistable lattices have been analysed with finite element method (FEM), and the solution was compared to the experiment. The bistable structure is composed of sinusoidal curved beams, vertical straight beams which connect curved beams with each other, and horizontal straight beams which cross the vertical beams. The bistability is exhibited by a sinusoidal curved beam snapping through from the initial state to a different state [2]. We designed the bistable lattices with straight beams of various widths and investigated how the straight beams affect the bistability. Specimens were fabricated by material extrusion (MEX) with thermoplastic polyurethane (TPU). The deformation of the specimens was recorded with a video camera during loading and during the unloading process, and the behaviours were compared to FEA simulation. When the straight beams were thin, the deformed state was unstable and shape recovery similar to superelasticity occurred since because thin straight beams bent greatly and could not restrain the deformed state of the sinusoidal beam. On the other hand, when the straight beams were sufficiently thick, although the curved beams deformed greatly, the deflection of the straight beams were small, and the deformed state was stabilized. We are going to propose a method of designing a cell lattice structure which exhibit these behaviours according to the required characteristics.

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Harnessing Distinct Deformation Modes of Auxetic Patterns for Tailoring Elastic Wave

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Key Words: *Auxetic, Elastic Wave, Bandgap, Disk Stiffness*

Auxetic metamaterial has a negative Poisson's ratio that expands laterally via a unique deformation mode induced by its internal geometry. Under shear, this metamaterial deforms similar to non-auxetic materials. This load-dependent deformation mode can be exploited to independently adjust structural properties in two different directions, for example, bending and torsional stiffness [1].

In this study, we introduce this concept to independently tailor elastic waves in two different modes, a flexural and torsional wave by adjusting their bandgap. To demonstrate it, a circular pipe structure with periodically arranged auxetic disks is considered. We designed auxetic disks with independently tuned torsional and radial stiffness in a wide range, validated by finite element analysis. The natural frequencies of each mode are then calculated, which determine the bandgap formation. The numerical measurements demonstrate that the elastic wave is prohibited to propagate in the bandgap, verifying that the wave propagation characteristics of two different modes can be independently tailored.

This work provides an integrated method that can independently design dynamic properties of two different modes which were inherently coupled, and has a potential to be applied in the field of vibration suppression and non-destructive testing.

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Thermally induced Phase Transforming Cellular Material using bimetal

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Key Words: *Phase Transforming Cellular Material, bimetal, finite element method*

Typical Phase Transforming Cellular Material (PXCM) are bistable metamaterials that undergo large displacement and are associated with the change in their periodic internal structure when a compressive load above a certain level is applied causing buckling of the curved beam [1,2]. Due to the bistability, such a PXCM maintains the deformed shape even after unloading and recovers the original shape by reverse deformation. However, the PXCM does not recover its shape unless tensile stress is applied. On the other hand, bimetal, composed of two metals with different thermal expansion coefficients, generates internal stress due to thermal strain and bends with temperature change [3]. If bimetals are incorporated into a part of the PXCM, it is expected that the PXCM will not only deform under compressive and tensile loads but also change its shape by heating and cooling. The purpose of this study is to fabricate a Thermally Induced PXCM (TIPXCM), which recovers its shape by temperature change after compressive deformation and exhibits pseudo shape memory property by using bimetals in the curved beams of PXCM. The optimum shape of the TIPXCM was designed by analyzing the deformation behavior under compressive loading and heating using the finite element method (FEM). Experiments were conducted using the fabricated TIPXCM, and the deformation associated with temperature change was measured using a high-speed camera and image analysis software to evaluate the relationship between temperature and strain.

As a result of the simulation, plastic deformation due to stress concentration was predicted to occur at both ends of the beam. To solve this problem of stress concentration, we designed a lattice structure consisting of bimetal beams whose ends were simply supported. The relationship between temperature and strain was measured by heating and cooling experiments on a half-unit cell of TIPXCM. The half-unit cell rapidly contracted at around -135°C and rapidly expanded at around 167°C owing to the snapping of the bimetallic beams, which are characteristic of this metamaterial. Then, we constructed TIPXCMs by arranging the unit cells. When the TIPXCM was heated, snap-through occurred in a step-by-step manner. The first snap-through triggered a chain reaction of deformation in other parts, and finally, the TIPXCM recovered more than 20% of its strain. This is more than twice as large as the strain recovery of Ti-Ni shape memory alloys (7-8%). This is a unique property of TIPXCM.

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Advanced discrete element method towards a digital twin based powder system

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Keywords: *Discrete Element Method, Cyber-Physical System, Digital Twin*

Nowadays, the development of a digital twin has received more attention in industries. This trend is no exception in powder industries. Towards the realization of a digital twin for a powder process, advanced modeling and simulation have been tackled. Therein, the discrete element method (DEM) [1] will be extensively employed. In my group, several key technologies for the DEM have been developed to construct the digital twin. The Signed Distance Function (SDF) [2] is useful to create the arbitrary shape wall boundary, even when the DEM is applied to the solid-fluid mixture systems [3,4]. The coarse-grained DEM [5] makes it feasible to simulate industrial powder systems efficiently. The geometrical approximation-based capillary force model [6] is shown to be effective to simulate industrial wet-particle systems. These technologies are integrated as an in-house code referred to as FELMI [7-9]. In this presentation, I will talk about the recent progress of the FELMI code and its application for the digital twin.

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DEM simulations of powder mixing in a pot blender

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Key Words: *Discrete element method, Pot blender, Mixing mechanism, Velocity gradient*

Powder mixing is widely employed in mineral, ceramic, nuclear and pharmaceutical engineering. To achieve an efficient mixing process, various type of mixers has been developed. A pot blender with both blending and storage capabilities offers an advantage over a conventional rotating drum. Unlike a typical rotating drum, the pot blender can simultaneously rotate and swing in controlled amplitude and frequency. Since the powder mixing in the pot blender is significantly influenced by the operating conditions and physical properties of the raw powder, the mixing operation of the pot blender has not been established so far. Therefore, in this study, we aim to elucidate the mixing mechanism of the pot blender using the discrete element method (DEM) [1] with a wall boundary model based on the signed distance function [2], which has been validated in the pot blender system [3]. Simulation results show that the mixing mechanism of the pot blender is mainly convective mixing in the rotational direction and shear mixing in the axial direction. Besides, as shear mixing in the axial direction become stronger due to the swing of the pot, diffusive mixing is suggested to intensify because the granular temperature increases with the variance of the axial particle velocity. A systematic series of simulations reveal that the velocity gradient in the axial direction, which mainly determines the axial mixing performance, is unaffected by particle density. Namely, the particle density has an insignificant influence on the mixing mechanism in the pot blender. Considering the relationship between the variance of axial particle velocity and granular temperature, the particle filling ratio is shown to significantly influence the mixing efficiency in the pot blender. Besides, dependency of the shear and diffusive mixing on Lacey's mixing index in the pot blender is newly clarified [4]. Consequently, the present study demonstrates novel insights into the mixing mechanism of the pot blender and comprehensive findings on the effects of particle density and particle filling ratio on the mixing process in the pot blender.

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DEM-CFD Simulation on Powder Mixing in a Tote Blender

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Key Words: *DEM-CFD, Tote Blender, Particle mixing, Air effects*

Homogeneous mixture of powders is in great demand for industrial products and produced through different kinds of mechanical mixers. Tote blender [1], widely used in pharmaceutical industry, has received scant attention in academic field. On the one hand, the features of flow regimes inside it have not been clearly studied. In addition, it's noted that air drag force acting on relatively small particles is not negligible during particle mixing [2], which is however not examined in tote blender hitherto.

By our in-house DEM-CFD method named FELMI [3], a reliable tool to simulate gas-solid flow, this study investigated the effects of air on particle mixing in a tote blender for the first time. To obtain comprehensive understanding, different rotation speeds (flow regimes), filling levels and particle sizes were involved. By visualization of flow regimes and evaluation of mixing state, the underlying air effects were analysed in detail. It's found that the mixing performance of small particles was significantly improved compared with that of larger ones in terms of Lacey's mixing index, since the air drag force changed the flow behaviour of small particles. More importantly, this pattern was observed in all the operating conditions, proved to be a universal rule.

This work provides novel insights about the prominent functions of air on mixing in the tote blender. It also conveys an import concept that air effects cannot be ignored when particles are small, which should be carefully considered in all the tumbling blenders.

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Development of DEM Based Blast Furnace Bell-less Top Model and Its Application in Burden Distribution

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Key Words: *DEM, Blast Furnace Bell-less Top, Burden Distribution*

Blast furnace is a large chemical reactor that is predominantly used for ironmaking purpose. Burden distribution plays an important role in achieving stable and efficient operation in a modern ironmaking blast furnace. Charging materials, e.g. coke and pellets, flow from upper hopper through a rotating chute and are distributed on the burden surface. The surface profile formed affects the gas flow distribution and particle descent behavior inside the blast furnace shaft. In present work, the authors proposed a DEM based numerical model to predict the burden distribution in a blast furnace and studied various aspects of burden distribution, including: falling trajectory of material, development of the burden profile at the throat, coke collapse, size segregation, and the gas velocity distribution across the furnace radius. Furthermore, the authors had tried to utilizing the burden distribution, thus gives a continuous production from the furnace as well as increase in the gas contact efficiency and a decrease in the energy consumption.

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Particle shape-induced radial and axial segregation of granular flow in a rotating drum

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Key Words: *Granular flow, segregation, rotating drum, ellipsoids*

Rotating drums are widely used in industry for mixing, milling, coating and drying processes. Particle mixtures with different physical properties in the rotating drums could segregate in the both radial and axial directions from an initially well-mixed state. In this presentation, we report the segregation phenomenon induced by particle shape. Particle shape used in our work is spheroidal which can be described by the parameter of aspect ratio (AR) defined as the ratio of both principal diameters of spheroids. Aspect ratio varies within a large range representing from oblate (AR<1) and spherical (AR=1) and problate shapes. Binary mixtures of spheres and spheroids are used in the discrete element method (DEM) simulation, and the segregations in both radial and axial directions are investigated. The results show that in a short drum, particle shape difference can cause radial segregation, but the segregation patters such as the locations of spheres and spheroids vary with the magnitude of the shape difference. With particle shape difference increasing, the segregation patterns could totally be reversed which can be explained by the reduced diffusion mechanism. For a long drum, the results show that for spheroid-sphere mixtures, spheres tend to segregate axially to the middle section of the drum, particularly for spheroids at aspect ratios = 0.67 and 2.0. The analysis reveals that the frictional end walls and the segregation developed in the radial direction induce the axial flow of particles, and are essential for the development of axial segregation.

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Systematic Phase-field Lattice Boltzmann Simulations to Investigate the Coherency Point in Semi-solid Deformation

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Key Words: *Semi-solid Deformation, Solidification, Phase-field Method, Lattice Boltzmann Method, GPU computing*

Semi-solid deformation occurs during casting with external forces of alloys. When the solid fraction exceeds a coherency point where grains impinge and a continuous network of grains becomes coherent, the semi-solid material exhibits a rheological behavior, which causes Reynolds dilatancy, such as in soil [1]. As the Reynolds dilatancy in semi-solid deformations causes serious solidification defects such as band segregation, pores, or cracks, identifying the coherency point based on various solidification conditions is critical.

Previous studies [2, 3] have reported that the crystal morphology, solid fraction, and deformation rate in semi-solid deformations are dominant for the coherency point. However, systematic investigations of these various factors have yet to be performed. To enable these investigations, numerical studies are indispensable. Still, no numerical models exist that can accurately express a multi-physics problem in semi-solid deformations, including solid–liquid transformation, fluid flow, and the motions and collisions of solids. In our previous study, a polycrystalline solidification model coupled with a multi-phase-field method, lattice Boltzmann method, and equations of motions of solids (which we termed a multi-phase-field lattice Boltzmann model) was successfully applied to a case of semi-solid deformation [4].

In this study, the multi-phase-field lattice Boltzmann method [4] was used to conduct systematic simulations of semi-solid deformation of an Al-Cu alloy under various conditions by changing the crystal morphology, solid fraction, and deformation rate. We investigated the effects of these factors on the coherency point through these simulations. The simulations for semi-solid deformation were accelerated by parallel computing using multiple graphics processing units.

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Atomic-scale Modelling of Chemo-mechanical Contributions to the Performance of Solid-State Batteries

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Key Words: *Microstructure, transport, mechanical properties, batteries, structure-property relationships*

Atomic scale calculations at the classical and quantum scale are used to probe how chemo-mechanical phenomena impact the performance of solid state batteries. Microstructure and mechanical properties of the solid electrolyte, metal anode, and the interfaces between them are considered. Phenomena that are investigated include the elastic properties of the bulk materials, local softening of elastic properties in the vicinity of grain boundaries, ideal strength, transport along grain boundaries, and interfacial adhesion. These properties are connected to failure modes associated with battery operation, such as void formation and dendrite nucleation at the electrode/electrolyte interface. These analyses reveal design guidelines for microstructural properties that enable robust battery operation.

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Catalytic Performance Affected by Hydrogen Spillover Mechanism: A DFT Study

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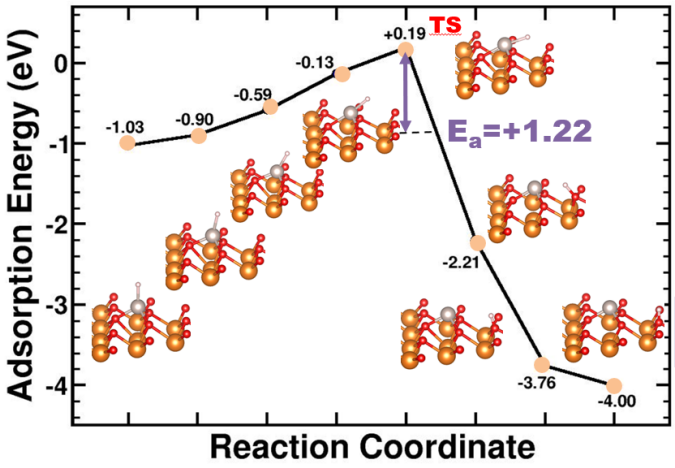
Key Words: *Ru/MgO, catalyst, hydrogen spillover, metal-support interaction, DFT*

Density Functional Theory (DFT) based electronic structure calculations have been used widely in modern Materials Science, Chemistry and Physics to disclose profound mechanisms of interest. Catalysts play a critical role in these energy conversion and storage technologies via enhancement of reacting rate, efficiency, selectivity of the relative chemical transformations. DFT can assist in understanding their mechanisms, improving material designs and predicting their performance. Here, I will focus on the correlation understanding between the hydrogen spillover mechanism and some catalytic reactions such as ammonia synthesis for future energy carrier application. First, we analyze the molecular or dissociative adsorption of on a single Ru atom as a benchmark or reference. Secondly, we analyze the binding energies between Ru-MgO(111) to understand their metal-support interactions. Thirdly, we would like to understand the physisorption and chemisorption of H_2 on MgO(111) supported Ru catalysts. Fourthly, we gradually adsorb more and more hydrogen atoms on Ru/MgO catalyst and attempt to understand the condition of triggering the occurrence of the phenomena of hydrogen spillover. The role of the supported metal particle is essential as it favours the spontaneous dissociation of H_2, a process that could rarely occur on the bare oxide surface without surface modification. However, MgO(111) seems to be capable of dissociating H_2 molecule. In this system, hydrogen spillover is not necessary to occurs at high hydrogen saturation conditions. Finally, we aim at correlating metal-support interaction with hydrogen spillover to quickly predict the catalytic performance and catalyst designs to reduce hydrogen poison problems or increase more active sites.



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Digital Twin of Battery Manufacturing Processes

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Key Words: *Rechargeable batteries, manufacturing process, digital twin, multiscale modelling, machine learning*

Lithium ion batteries (LIBs) are a very important technology for our societies. Their performance is strongly influenced by the mesostructure of their porous electrodes. This mesostructure results from a complex process encompassing multiple steps and numerous parameters. Its understanding and accelerated optimization is vital for the future of battery technology.
In this lecture I discuss a digital twin for accelerated optimization of the manufacturing process of LIBs we are developing within the context of the ARTISTIC project.[1,2] Such digital twin is supported on a hybrid approach encompassing a physics-based multiscale modeling workflow, machine learning models and high throughput experimental characterizations. Different steps along the battery cells manufacturing process are simulated, such as the electrode slurry, coating, drying, calendering and electrolyte infiltration. The multiscale physical modeling workflow couples experimentally-validated Coarse Grained Molecular Dynamics, Discrete Element Method and Lattice Boltzmann simulations and it allows predicting the impact of the process parameters on the final electrode mesostructure in three dimensions. The predicted electrode mesostructures are injected in a continuum performance simulator capturing the influence of the pore networks and spatial location of carbon-binder within the electrodes on the solid electrolyte interphase formation (for anodes) and the electrochemical response (of anodes vs. lithium, cathodes vs. lithium and the full cells). Machine learning models are used to accelerate the physical models' parameterization, to mimic their working principles and to unravel manufacturing parameters interdependencies from the physical models' predictions and experimental data, and as a guideline for reverse engineering. The predictive capabilities of this digital twin, coupling physical models with machine learning models, are illustrated with results for different electrode formulations. Finally, the free online battery manufacturing simulation services offered by the project[3] and our virtual reality technology supported on the project results to optimize battery electrodes and for the project results dissemination are illustrated through several examples.

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Energetics and Dynamics of Lithium Intercalation in Graphite from Machine Learning-based Energy Model

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Key Words: *Atomistic Simulation, Machine Learning, Lithium Intercalation, Graphite*

Graphite has been widely used as the anode material of commercial lithium ion batteries for almost three decades. Recent studies have indicated that the capacitance of Li-graphite anodes could reach beyond the theoretical magnitude of 372 mAh/g, suggesting that there still lacks comprehensive, atomistic insights into the detailed intercalation energetics and dynamics of lithium intercalation into graphite. Herein, a hybrid machine learning (ML) energy model combining the spectral neighbor analysis potential (SNAP) and the dihedral-angle-corrected registry-dependent (DRIP) model were trained for Li-graphite system. A number of high lithium intercalation density configurations, including LiC_2 and multi lithium layer intercalation in conjunction with different graphite stacking types were taken into account in the training set, allowing us to explore the true upper limit of lithium intercalation into graphite. The trained hybrid ML energy model allows us to perform extensive large-scale atomistic Monte Carlo sampling of lithium intercalation into graphite, while retaining high fidelity in potential energies and atomic forces prediction with respective density functional theory (DFT) calculations. Our simulation results suggest that during thermodynamic equilibrium condition, it is highly likely that the actual capacity of Li-graphite anode is much higher than that of LiC_6; however, it is very difficult to attain due to the constrain imposed by lithium diffusion kinetics.

Modeling and Simulations of the Structure and Lithiation Mechanism of Silicon Oxycarbide Ceramics

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Key Words: Li-ion Batter, Silion Oxycarbide Ceramics Glass, First-Principles Calculations, ReaxFF Modelling

Silicon oxycarbide (SiOC), a polymer-derived ceramic, is considered as a promising anode material for the next generation lithium ion batteries primarily owing to its excellent electrochemical and cycling performance during the lithiation and de-lithiation processes. However, the structure characteristics and the lithiation mechanism of silicon oxycarbide remain very controversial and unclear yet to date. In this study, we employed *ab initio* molecular dynamics simulations to generate the structure models of amorphous silicon oxycarbide within various chemical compositions ($SiC_{3.3}O_{1.6}$, $SiC_{2.2}O_{1.6}$, $SiC_{1.65}O_{1.6}$, $SiC_{0.8}O_{1.6}$, $SiC_{1.65}O_{1.1}$, $SiC_{1.65}O_{0.6}$) and then investigate the atomistic mechanisms of the Li-ion intercalation as well as the origin of the huge capacity loss upon the 1st cycle of lithiation. Our results first revealed that the C atoms are very likely to segregate out and form the graphitic-like free C phase within the remaining SiOC glass in the amorphous material bond network. As the C/O ratio is low, the free carbon atoms may simply form fragmented amorphous graphene layers in the composite material bond network, while they can turn into the multi-layer disordered graphene phase as the C/O ratio is much further increased. Based on those SiOC structure models generated, their lithiation mechanisms were found to exhibit a very interesting and distinct intercalation behavior from other anode materials considered. During the early stage of lithiation, the intercalated Li ions were mainly located at the interfaces between the SiOC glass and the free C phase. Our charge density analysis further showed that the electrons were mainly accommodated by the free C phase while the Li ions were predominantly adsorbed on the O atoms of the SiOC glass. During the 2nd stage of lithiation, the Li ions started to migrate into the SiOC glass region and sequentially break the Si-O bond networks. Upon the end of lithiation, the Li storage capacity of the silicon oxycarbide anode was found to be within the range between 800 and 1200 mAh/g, in good agreement with the recent experiments. Our simulation results further revealed that the Li storage capacity and the irreversible capacity loss in the 1st cycle of lithiation are largely determined by the C content in the silicon oxycarbide anode. A detailed explanation of the underlying physics and the associated atomistic lithiation mechanisms of the silicon oxycarbide anode will be addressed in this presentation.

Theoretical Insights Toward Alleviating Lattice-Oxygen Evolution in Li-rich Layered Manganese Oxide Cathode Materials

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Key Words: *$LI_{1.2}NI_{0.2}MN_{0.6}O_2$, OXYGEN EVOLUTION, AIMD*

Recently, Li-rich layered manganese oxide-based cathodes have drawn much attention for the next-generation lithium-ion batteries due to the large discharge capacities and low cost. However, the lattice oxygen release and subsequent surface densification during cycling inevitably lead to their instability, which incurs capacity failure at high voltage. Improving the stability of lithium-rich cathode materials is important in refining the overall performance of lithium-ion batteries. In my presentation, I will show the mechanism of lattice oxygen evolution and related electronic properties of $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$ (LNMO) cathode materials.[1,2] Then I will illustrate the lattice oxygen release in LNMO cathode surface can successfully suppress through the doping using density functional theory (DFT) calculations and ab initio molecular dynamics (AIMD) simulations.

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Investigation on Characterization of Force Chain Structure using Discrete Element Method

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Key Words: discrete element method, non-Bagnold flow transition, force network community, force chain duration time

A granular flow is the collective motion of discrete solid particles and its continuum modeling has challenged researchers for decades due to its multiphasic flow characteristics, especially at the solid-liquid phase transition. This is because the interaction mechanisms among the constituent particles may have changed from repulsive binary collisions to enduring frictional contacts with multiple neighbors, leading to the formation of force chain structure. This chain-like structure forms an internal network to transmit momentum more effectively than collision-induced transport and hence is worth investigating how the flow behavior changes accordingly. On the framework of discrete element simulation, we implemented two algorithms to extract the force chain structure in a steady granular flow. The first approach uses the depth-first search to identify force chains in a plane shear flow. Statistical data of the length and the lifetime of the longest chain shows monotonic decrease with the flow inertial number, I. A lower I indicates a more solid-like flow state and the finding confirms the speculation that the force chains also develop to a wider spatial extent. The second approach implements the Louvain greedy algorithm to identify force chains as network communities and the number of force chain disks is evaluated across the depth of surface granular flows of different heights and inclinations. The statistics shows that more disks are engaged to develop force chains in deeper layer and such depth-variation is only noticeable when the flow is more solid-like with a sufficiently low Froude number. With decreasing Froude number, the force chains carry a growing portion of the flow internal stress but an upper limit around 0.6-0.7 is consistently detected. The most intriguing finding reveals that the sudden rise of force chain disk number and their carried stress portion is linked to a degradation of flow velocity profile from the Bagnold profile, known to exist when collision is the primary interaction mechanism.

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Simulations of Granular Flow Behaviors and Mixing Process in Fluidized Bed Mixer

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Key Words: *Fluidized Bed, Additive Manufacturing, Granular, Mixing, Two-phase Model*

As per ASTM, additive manufacturing (AM) is defined as the process of joining materials to fabricate objects from 3D-model data (typically layer upon layer), as opposed to subtractive-manufacturing methodologies [1]. Although AM has been used as a material-processing method for more than 20 years, it has only recently been considered an important commercial manufacturing technology. The AM process can involve var- ious materials such as metals, ceramics, or composites. However, metal products are most widely used in industrial applications.

A significant portion of the operating costs of commercial AM equip- ment is due to the metal powders used in the AM process. The fine metal powder that is used for laser melting is expensive, and thus it is important to avoid any wastage. In most cases, only a small portion of the powder that is placed on the bed is actually soldered into a component. Most of the powder is not melted, and is thus available for re-use. However, the recycling powder have to be mixed with the fresh powder in the final step before it can used to the next process. The segregation phenomena is a common problem in the mixing process or transportation process. Therefore, it is importantly to understand the theory and the mechanism of powder segregation/mixing, and to reduce the probability of occurrence. Powders can be mixed by mechanical excitation, gas-flow agitation, gravity-driven free-falling, and many other different complex methods [2]. The mechanisms of powder mixing include convective mixing, shear mixing and diffusive mixing [3-5].

In this study, we performed numerical simulation to investigate gas-solid interaction problems in a fluidized bed powder mixing system, in which a coupled CFD-DEM method was used to investigate the mechanism of gas flow and the particle tracking for granular flow. In the DEM, Lagrangian particle tracking method was employed to calculate the particle motion. CFD analysis by using Eulerian model was used for the determination of velocity and pressure field for the gas phase. we analyzed the velocity and pressure changes of the fluid field. Next, we also investigate the trajectory, velocity and granular temperature of the granular powder, and analyzed the mixing intensity with time revolution and mixing rate by using the mixing index. It showed that both the gas velocity and the inclined angle of air inlet affect the mixing rate and mixing degree.

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The mechanism for hopper flow rate enhancement by an optimally-placed obstacle

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Key Words: *Granular Materials, Jamming, Tetris-like Model, Discrete Element Method*

How to enhance the discharge flow rate of granular particles moving through a hopper under the influence of gravity is an important engineering and industrial question. Surprisingly, an optimally placed obstacle in a hopper allows particles to exit the hopper more efficiently, similar to how proper placement of traffic signals and signs can improve traffic jam. An obstacle placed too far from the hopper exit allows so many particles to pass that they are prone to congest as they are funneled together. An obstacle placed too close lowers the chance of congestion at the exit but allows so few particles to pass that it reduces overall flow. An optimally placed obstacle creates a flow rate enhancement by channeling the maximum number of particles that can smoothly merge. Using a novel modeling technique that simplifies the complications of interparticle forces, we show that this phenomenon can also be created by either artificially guiding the particles into the free space under the obstacle or by narrowing the hopper exit angle below the obstacle. These findings can be used in the design of hoppers that discharge granular particles more efficiently and we expect them to have broad industrial applications.

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2D mesoscale approach for modeling concrete fracture under uniaxial compression using the mesh fragmentation technique

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Key Words: *Mesoscale Model, Mesh Fragmentation Technique, Uniaxial Compression, Concrete.*

Even nowadays it is still a challenge to predict numerically the failure behavior of concrete under compression. Multiscale models have been used to better understand the influence of the distinct phases of the concrete on the fracture process. In this sense, this work proposes an extension of the mesh fragmentation technique developed by Manzoli et al. [1] to account for the complex failure behavior of concrete under compression. The concrete is represented using a mesoscale approach, as proposed by Rodrigues et al. [2], however, the pairs of interface elements inserted into the standard finite element mesh to define the potential fracture paths are duplicated to describe the compressive failure as a combination of tensile and tangential constitutive models.
The use of these two damage models makes it possible to represent the debonding (opening) between the aggregates and matrix due to local tensile stress concentration, i.e. the fracture propagation in mode I, as well as the sliding process that corresponding to the fracture propagation in mode II. Furthermore, adopting adequate parameters, these models even allow representing the friction condition between the concrete specimen and the steel loading plates. Numerical examples assuming different specimen slenderness as well as the different friction restraints between loading platen and concrete specimen are carried out. The numerical results are compared qualitatively and quantitatively against the experimental results found in the literature [3], demonstrating the proposed approach is promising to describe the failure process of concrete in compression.

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Determining upper and lower bounds to the elastic threshold for problems of dissipative strain-gradient plasticity

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Key Words: Strain-gradient plasticity, dissipative theory, duality, finite element method, upper and lower bounds

Strain-gradient plasticity refers to a class of extensions of classical elastoplasticity in which size-dependent effects are accommodated through the introduction of a length scale together with gradients of plastic strain. The area has received sustained interest, with multiple theoretical, experimental and computational contributions (see for example [1] and the references therein).

Strain-gradient theories are generally energetic or dissipative in nature. The former refers to models in which the plastic strain gradients are incorporated in a defect energy, while in the latter model the plastic strain rates and their gradients are determined through an extension of the classical associative flow relation and a yield function that depends on microstresses, which are not known in the elastic region.

This presentation focuses on the dissipative version of rate-independent strain-gradient plasticity, for which yield and plastic flow must be considered at the global level. This is a generally intractable problem, and so it is useful to develop methods for approximating yield. One such approach is discussed here: it draws on the methods of limit analysis together with primal and dual versions of the global problems, to establish conditions for lower and upper bounds to the elastic threshold. The approach is illustrated through various examples, using a computational approach with penalization.

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Modeling fluid flow in vuggy porous media using coupling finite elements

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Key Words: Coupling finite elements, Vuggy porous media, Non-matching meshes

Studying the characteristics of rock formations is of great importance in a number of engineering applications, such as geothermal energy extraction, nuclear waste storage, CO_2 sequestration, and oil and gas extraction [1]. In terms of hydraulic analyses, the presence of geological features such as fractures, vugs and barriers can significantly affect the equivalent permeability of the porous medium [2], but modeling vuggy fractured porous media is still a challenging problem, since the geometry of fractures and vugs are very complex and involves several dimensions and arrangements. In this context and based on the finite element method, conventional meshes require a significant computational effort when dealing with problems with multiple scales, since many transition elements are required to smooth the transition between the dimensions. This work proposes to model each geological structure completely independent from each other (i.e., in a non-matching way) and couple them in the porous medium mesh by means of coupling finite elements (CFE). The CFE can be inserted during the pre-process stage and does not add new degrees of freedom to the system of equations [3]. The technique was applied in 2D single-phase flow problems in vuggy fractured porous media, with incompressible fluid. To verify and validate this technique, the results were compared against the ones obtained with conform meshes, which were used as reference. Based on this comparison, a good similarity was observed between the responses, as well as a significant reduction in the number of elements used to discretize the problem. The effects caused by fractures that act as barriers (fracture less permeable than the porous media) were also captured.

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Plasticity without phenomenology: a first step

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Key Words: Temporal multiscale, Plasticity, Dislocation Dynamics

This talk aims to understand and exploit the slow time-scale behavior of rapidly evolving microscopic dynamics. The microscopic systems considered are posed in terms of systems of non-linear ordinary differential equations, not necessarily containing an a priori split into fast and slow variables. Such a question arises naturally and ubiquitously in efforts to understand macroscopic dynamics, on engineering time-scales, of well-accepted models of microscopic dynamics that, however, are not amenable to practical computing over the much, much larger macroscopic time-scales of interest. This is because there is a vast separation of time scales involved between the dynamics of the macroscopic variables of interest and the microscopic dynamics, and evolving the microscopic dynamics directly fails to address the question of the macroscopic dynamics.

The methodology employed involves a computational scheme based on fundamental mathematical theory that a) defines appropriate `coarse' variables corresponding to the microscopic dynamics that evolve in a stable manner on the coarse time scale; b) determines the equation of evolution for such variables; and c) defines a practically useful strategy for accurately initializing short bursts of microscopic runs for the evolution of the slow variables, without special requirements on the nature of the microscopic dynamics.

We will illustrate the theory with examples that violate ergodicity and include both conservative and dissipative behavior. The coarse graining of discrete dislocation dynamics to a pde-based plasticity model without relying on constitutive assumptions will also be demonstrated.

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An efficient multiscale homogenization modeling approach to describe elasto-plastic behavior of polymer nanocomposites

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Key Words: *Polymer nanocomposite, Interphase, Multiscale modeling, Plastic deformation*

In this study, we proposed the multiscale bridging approach to describe the elasto-plastic behavior of polymer nanocomposites by combining the molecular dynamics (MD) and finite element (FE) homogenization method. It has been reported that the precise characterization of interphase elasto-plastic constitutive law is critical in the prediction of the fracture toughness and fatigue crack growth behavior [1] as well as the strength of polymer nanocomposites. Yang et al. [2] developed the multiscale bridging approach to elasto-plastic behavior of polymer nanocomposites including the carbon nanotubes by combining the molecular dynamics (MD) and micromechanics theory. However, the multiscale bridging method based on the MD and FE homogenization method has not been developed. Because the FE homogenization method is more accurate than the analytic micromechanics solutions, it is critical to develop the multiscale bridging method based on the MD and FE homogenization method to describe the elasto-plastic behavior of polymer nanocomposites. We have used a three-phase continuum homogenization model, which include the interphase zone as well as the matrix and particle. The interphase elasto-plastic properties are inversely obtained by the MD and FE homogenization method. For various nanoparticulate size, the interphase properties obtained from the proposed method are compared with those of the multiscale bridging method based on the MD and analytical mean-field homogenization (MF) method. Furthermore, for the efficient characterization of the interphase elasto-plastic constitutive law, the proper orthogonal decomposition (POD) is applied.

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Computational hygroelastic aging study of cross-linked epoxy-based nanocomposite

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Key Words: *Epoxy, Hygroelastic aging, Molecular dynamics, Diffusion*

This study demonstrates moisture uptake and hygroelastic degradation of epoxy-based nanocomposite using classical molecular dynamics simulation and Monte Carlo simulation. The hygroelastic aging is one of the representative aging caused by continuous exposure to humid environment. Water molecules absorbed inside epoxy and epoxy-reinforcement interface act as a plastisizer to decrease elastic modulus of cross-linked network. Moreover, anchored moisture occupying the free volume in epoxy result in swelling and eigenstress. Therefore, we performed a systematic combinatory simulation of moisture transport and resultant hygroelastic aging of epoxy-based nanocomposite. Considering the humidity of epoxy's service condition moisture uptake was studied by using a Monte Carlo simulation. From the moisture content-volumetric expansion relation, the swelling coefficient of nanocomposite was determined. According to the moisture content, the elastic modulus of nanocomposite was determined from uni-axial tension test. To study the degradation of epoxy-nanocarbon interface by the moisture invasion, simple laminated unit cell model was constructed. From mode1 and mode2 decohesion test, normal and tangential cohesive law was determined according to the hygroelastic aging. Finally a multi-scale hygroelastic constitutive model was proposed and sequentially bridged to the MD simulation results.

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Computational modeling to evaluate effect of the partial debonding on fracture toughness of polymer nanocomposite

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Key Words: *Fracture toughness, Polymer nanocomposite, interfacial debonding, Matrix plastic yielding, Finite element analysis*

Due to significantly improved properties and multifunctional behaviors by nanoparticles, intensive researches on nanocomposites have been performed. One of the most interesting features is the fracture toughness enhancement of the nanocomposite even at low filler concentrations. Many researchers [1,2] have developed theoretical models to predict the toughness enhancement of nanocomposites, considering the main toughening mechanisms such as the interfacial debonding, the plastic yielding of nanovoids and localized shear banding of the polymer. Zappalorto M et al. [2] proposed multiscale model base on the assumption that the interface between the polymer matrix and the particles is uniform. However, in the process of synthesizing the nanocomposite, It is impossible to generate unifom interface between the components, and voids could be generated without interfacial bonding force.

In this study, a computational modelling based on finite element (FE) analysis is proposed for analyzing the fracture toughness of silicon carbide (SiC)/epoxy nanocomposite. We intensively address energy dissipated by two mechanisms for toughness enhancement: interfacial debonding and the plastic yielding of nanovoids. A three phases nanoscale system (particle-interface-matrix) is modelled, and the analytical model proposed by Zappalorto M et al. [2] is applied to calculate the parameters for FE analysis such as critical debonding stress and extension of the plastic zone. Crack-induced stress at the macroscale is transferred into the nanoscale FE model through the scale-bridging method. The simulation results show that the dissipated energy of the plastic yielding of nanovoid increase nonlinearly as the specific debonding area increase, which proves that the interfacial partial debonding have a significant effect on the toughness enhancement of the nanocomposite. The proposed FE modeling approach is expected not only to overcome the limitations of the analytical model that cannot depict partial debonding, but also serve as a foundation for designing nanocomposites.

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Data-Driven Computational Mechanics of hyperelastic materials using MLP, GR and RBF models of Artificial Neural Network

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Key Words: *Neural network constitutive model; Hyperelastic model; Artificial neural network; Molecular dynamics simulation; Data-driven computational mechanics; two-scale finite element analysis*

Artificial neural networks (ANNs) are being applied in many research fields. Among them, the neural network constitutive modeling studies on nonlinear problems in the field of mechanical engineering are important. In this study, three different types of neural models: multi-layer perceptron neural network (MLPNN), generalized regression neural network (GRNN), radial basis function neural network (RBFNN) are used to construct neural network constitutive models (NNCMs) for hyperelastic materials. We focus on the two cases of ANN training of data set: (i) the conventional hyperelastic models such as the Mooney-Rivlin model, and (ii) full atomistic molecular dynamics (MD) simulation results. Here, we obtain the optimal hyperparameters empirically at each neural network modeling to construct optimal NNCM. These three models were compared based on statistical error analysis. The results indicated that RBFNN model is the most accuracy through RMSE, MAE, and R values. We apply the proposed NNCM model to the data-driven computational mechanics (DDCM) to verify the proposed NNCM model. Additionally, the data-driven two-scale finite element analysis framework is proposed by using the microscopic equilibrium equation solution data-driven ANN model with proper orthogonal decomposition method. As results, the data-driven solver shows the superiority of the performance of RBFNN model than the other neural network models.

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Effect of Heterogeneous Curing Temperature on Crosslinking Morphology and Mechanical Properties of Epoxy Thermoset Plastic: A Coarse-Grained Molecular Dynamics Simulation

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Key Words: *Coarse Grained Molecular Dynamics, Epoxy, Heterogeneous Curing Temperature, Mechanical Properties*

Because epoxy has excellent thermomechanical properties, it is used in various industries such as electronic, aircraft, automotive and composite materials. The excellent physical properties of the epoxy are due to the cross-linking network formed by chemical bonding between the epoxy resin and the crosslinking agent. Various studies using molecular dynamics have shown that factors such as crosslink density, crosslinking process, curing agent structure, and ratio affect crosslinking network formation [1-3]. According to a recent experimental report, the heterogeneous temperature during the crosslinking process forms a heterogeneous crosslinked network, which greatly affects the mechanical properties of the epoxy [4-6]. However, it is difficult to analyze the crosslinked network in detail with an experimental approach, and the analytical approach using simulation is also insufficient due to the limitation of the scale.

In this study, a computational model based on molecular dynamics is proposed for analyzing the effect of the heterogeneous curing temperature on crosslinked network and mechanical properties. We extended the length scale of the classical molecular dynamics model using Coarse Grained Molecular Dynamics (CGMD). And 10 cases of heterogeneous heating simulation were performed. The simulation results showed that the more heterogeneous the curing temperature is, the more heterogeneous the crosslinked network becomes. In the heterogeneous crosslinked network, area with a low crosslinking density was observed. This area was vulnerable to void formation, resulting in an early local yield, which consequently accelerated the yield of the material. The proposed CGMD modeling approach is expected not only to overcome the limitations of the classical molecular dynamics model that cannot depict heterogeneous curing, but also serve as a foundation for designing nanocomposites using epoxy thermoset plastic.

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Effect of nanoparticle agglomerations on the mechanical behavior of polymer nanocomposite: a coarse-grained molecular dynamics simulation

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Key Words: *Coarse-grained molecular dynamics, polymer nanocomposite, nanoparticle agglomeration, particle swarm optimization, artificial neural network*

As polymer nanocomposites have attracted significant attention over the years for enhanced thermomechanical, electrical properties and multifunctional behavior, many attempts have been made to analyze characteristics of polymer nanocomposites at molecular level using the molecular dynamics (MD) simulations [1, 2]. However, due to limitations of time and length scale resulting from atomistic-level calculations, the interaction between multiple nanoparticles could not be taken into account, and therefore the correlation between nanoparticle distribution and mechanical behavior of nanocomposites is still not fully understood.

In this study, we present multiscale simulation framework based on the coarse-grained MD simulations to investigate mechanical behavior of silicon carbide (SiC) / polypropylene (PP) nanocomposites. We adopted coarse-grained MD simulations as an effective tool for the advantage of maintaining the molecular details while extending time and length scale of simulation with less computational efforts. The new coarse-grained potential, composed of bonded and non-bonded terms, is derived through optimization process based on artificial neural network (ANN) assisted multi-objective particle swarm optimization (MOPSO) to fit certain key thermomechanical properties of SiC/PP nanocomposites obtained from full atomistic MD simulations. The predictions of coarse-grained model single nanoparticle and two nanoparticles are in very good agreement with reference data. Based on that result, we conduct uniaxial tensile deformations by varing polymer-nanoparticle and nanoparticle-nanoparticle interactions to deepen the understanding of microscopic mechanism of nanoparitcle distribution on stress-strain behavior The proposed multiscale simulation approach can elucidate effect of agglomeration of multiple nanoparticles on nanocomposites, and it can provide insight on efficiently designing the nanoparticle/polymer nanocomposites.

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Electroelastic Properties of SW defected h-BN Nanosheets studied by Molecular dynamics simulation

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Key Words: *Molecular Dynamics, h-BN sheet, Nanocomposites, Dielectric constant, piezoelectric constant*

In this study, Molecular dynamics simulation(MD) is used to investigate the Electroelastic properties of hexagonal crystallographically boron nitride nanosheets (h-BN nanosheets). Randomly generated Stone-Wales(SW) defect in h-BN nanosheets is considered in the simulation to reveal how the defect in h-BN affects the electroelastic properties. Based on the linear piezoelectric constitutive law, both reverse piezoelectric and direct piezoelectric simulation were implemented. In order to describe electroelastic behaviour of h-BN, several Tersoff potential models were applied. In reverse piezoelectric simulation, varying electric field was applied along the in-plane direction of h-BN and the resultant polarization and induced stress were used to determine the dielectric constant and the piezoelectric constant, respectively. In direct piezoelectric simulation, h-BN was mechanically elongated without electric field. From the strain-polarization and strain-stress relation, piezoelectric constant and young's modulus of h-BN were determined. As the SW defect increases, the dielectric constant increases as a result of relative electric displacement of boron and nitrogen atoms. On the other hand, the piezoelectric constant showed increasing as well as decreasing trend depending on the Tersoff potential model applied to the simulation. The Young's modulus was found to decrease as the number of SW defect increase regardless of the Tersoff potential model.

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Enhanced Lo-Christensen-Wu theory in Laplace domain for the Thermo-Mechanical-Viscoelastic Analysis of Laminated Composite Structures

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Key Words: *Laminated Composites, Thermo-Mechanical-Viscoelastic Analysis, Mixed Variational Theorem, Laplace Transformation*

Recently, composite materials have been widely used in various engineering applications due to their high stiffness-to-weight ratio and multifunctional characteristics. Although the laminated composite plates has a great structural performance, mechanical imperfections such as layer delamination can be induced by transverse shear and normal stresses. There are many theories developed to accurately predict these transverse stresses, such as the well-known conventional theories (FSDT; first-order shear deformation theory) and many other refined shear deformation theories (HSDT; higher-order shear deformation theory, EHOPT; efficient higher order plate theory, EFSDT; enhanced first-order shear deformation theory).

When the composite materials are used in severe operating conditions such as extremely high temperature environments, composite structures have thermal expansion as well as viscoelastic characteristics such as creep strain, stress relaxation because the matrix of composites become viscoelastic materials in high temperature environment. Thus, thermo-mechanical-viscoelastic effects of the laminated composite structures should be considered for the reliable analysis. As a way to address aforementioned issues, a new type of enhanced analysis model based on the Lo-Christensen-Wu theory (ELCW) in order to accurately predict the viscoelastic behaviors of laminated composite plates under thermo-mechanical loading. In the ELCW, the concepts of the strain energy relationship and Laplace transformation are employed in order to improve the solution accuracy and computational efficiency at the same time.

In this paper, thermo-mechanical-viscoelastic analysis using an enhanced LCW theory (ELCW) will be performed, and the results of the present theory will be compared to those reported in the open literature.

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Hyperthermal Erosion of Thermoprotective Nanocomposites Under LEO Environment: A Reactive Molecular Dynamics Study

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Key Words: *Low earth orbit (LEO), Atomic oxygen (AO) bombardment, Surface recession, Reactive molecular dynamicssimulation, Erosion yield*

Organic polymer-based nanocomposites incorporating nonvolatile inorganic nanoparticles or low-dimensional nanocarbons have long been studied for the spacecrafts and satellites aviating low earth orbit (LEO) and sub-LEO. Against the harsh oxidizing condition attributable for the hyperthermal atomic oxygen (AO) bombardment, mitigation of the surface recession and etching has been the main issue in designing surface shielding materials. In this study, systematic reacitve molecular dynamics (MD) simulations incorporting the reaxFF forcefield were performed to study the hyperthermal erosion of polyimide (PI)-based nanocomposites reinforced with highly thermoprotective inorganic nanofillers. In order to propose optimum reactive simulation condition to mimic the interaction between the nanocomposites surface blanket layer and colliding gaseus atoms or molecule in aviation condition of satellites in LEO, some boundary conditions and thermostatting were tested first. To enable well-developed and steady temperature profile inside the nanocomposites during the bombardment simulation, microcanonical ensemble simulation with a enough thickness of nanocomposites slab more than 4nm was proposed. To prevent the drift of the slab model, during the bombardment simulation, both reflection condition and geomteric constraint at the bottom of the slab models were found desirable.

To descibe the surface recession and temperature rising at the boundary between colliding gases and nanocomposites solid surface, AO particles were collided with a kinetic energy of 4.5eV which corresponds to a typical aviation speed of 7.4km/sec in LEO satellites. As thermoprotective nanofillers both planar and tubular nanostructures were embedded into the PI matrix with a random oritentation. During the bombarmdent simulation, the themperature riging rate and the erosion yield of the nanocompositesx were calculated. With all types of additives studied, a meaningful thermoprotection was achieved in erosion yield and temperature rising rate. Due to the unpaired electrons, AO bombardment showed a sequential disintegration of oxidation and desorption forming volatile oxides. The erosion yield determined from the present reactive MD simulation was compared with the reference value measured from MISSE experiment in international space station (ISS). In addition, the surface recession rate during the hypertmal erosion simulation was determined and corrected to the real aviation speed of the ISS. The corrected surface recession rate determined from the reactive MD simulation was comparable to the in-flight experimental result.

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Multiscale model to predict fracture toughness enhancement and fatigue crack growth behavior of polymer nanocomposites

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Key Words: *polymer-matrix composites (PMCs); nanocomposites; fatigue; fracture toughness; toughness mechanisms*

In this study, we develop the multiscale model for the prediction of the fracture toughness enhancement and fatigue crack growth behavior of the polymer nanocomposites (e.g., epoxy/SiC nanocomposites, epoxy/CNF nanocomposites). For the epoxy/SiC nanocomposites, we considered the three main toughening mechanisms (interfacial debonding, subsequent plastic nanovoid growth, and plastic shear band) [1]. For the epoxy/CNF nanocomposites, we considered the other three main toughening mechanisms (interfacial debonding, subsequent plastic nanovoid growth, and pull-out of the CNFs) [2]. To the best of my knowledge, this is the first attempt to develop a multiscale modeling framework by merging all-atomistic molecular dynamics (MD) simulations, micromechanics, and the linear fracture mechanics theory. The predicted fracture toughness and the fatigue crack gorwth of polymer nanocomposites are validated by the comparison with the experimental data. Furthermore, according to our parametric studies, it is clear that the fracture toughness of polymer nanocomposites are rapidly increased as the nanoparticulate diameter decreases.

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Multiscale simulation for understanding chemomechanics in layered-type cathode of advanced sodium-ion batteries

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Key Words: *First-principles calculation, Finite element analysis, Multiphysics, Sodium-ion batteries, Layered-type cathode*

Due to the lower standard redox potential of Na/Na^+, sodium-ion batteries (SIBs) have a limitation on the energy density.[1] To overcome this hurdle, using an anionic redox reaction of O^{2-}/O^{n-} has been highlighted for enlarging the energy density limit of SIBs. To use more energy density from the lattice oxygen redox, most of the sodium-ion needs necessarily to be extracted from the host material, which intrinsically accompanies a large lattice distortion resulting in the irreversible degradation of electrochemical performances.[2] To properly utilize the oxygen redox reaction for the energy density extension, an in-depth understanding of the structural distortion in the primary particle and its effect on the secondary particle is necessary.
In this study, we conduct first-principles calculations to evaluate the lattice change of layered-type $Na_{1-x}[TM]O_2$ in the primary particle. Based on that result, we demonstrate the sodium-ion diffusion and corresponding mechanical behavior in the secondary particle. When the sodium-ions are heavily extracted, layered active materials undergo an abrupt lattice contraction along the out-of-plane direction, which is an inevitable mechanical distortion for layered cathode active materials. This abrupt and anisotropic lattice change causes intergranular damage for the normal secondary particle, resulting in the capacity fading. Therefore, it is important to design the secondary particle that can withstand the structural distortion in the primary particle for enhancing cycle life. Based on the first-principles calculations and the finite element analysis, we give insight into the morphology of the secondary particle to properly withstand the effect of the primary particle lattice distortion.[3]

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Polymer pyrolysis modelling by coarse-grained molecular dynamics: A parametric study

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Key Words: *Polymer Pyrolysis, Coarse-grained Molecular Dynamics, Bond Breaking*

Polymer materials can be studied computationally by all-atom (AA) molecular simulations such as molecular dynamics (MD) at a temporal and spatial scale within 100 ns and 10 nm, respectively. In practice some reactive degradation of composites including pyrolysis can take place in much larger scales. For example, due to limitation of time scale, AA MD requires higher temperature for the pyrolysis process to happen in comparison with experimental data [1]. A possible way to extend molecular modelling and bridge it with macroscale computational and experimental techniques is to use coarse-graining: represent a large molecular system efficiently by a reduced number of degrees of freedom. In this study we demonstrate a coarse-grained MD simulation (CGMD) on the pyrolysis of polymer networks under high temperature and atomic oxygen (AO) bombardment.

Polyethylene is considered as an example material for the development of CGMD simulation model with a mapping ratio of 2:1, i.e., two CH_2 groups are represented by one equivalent bead. The CG interaction is described with the DREIDING force field including bonded, angular, torsion and vdW interactions. The bonded interaction can be either Lennard-Jones potential in equilibrium process or Morse potential in pyrolysis process. For the pyrolysis or thermal degradation of polymer networks, the bond breaking phenomenon is implemented in the simulation model, with a criterion based on the critical energy or length of the bond. Because the release of two particles of a broken bond can cause significant disturbance to the system energy, the particles related to bond breaking are relaxed separately with a limited maximum movement.

The parametric studies are performed to investigate the effects of modelling parameters of bond breaking, individual interaction potential, characteristics of oxygen bombardment, etc for the structure-to-property relationship. The results have verified qualitatively that CG MD with bond breaking can be used to capture the pyrolysis process of polymeric systems under hyperthermal reaction condition. In AO bombardment simulation, the energy exchange between gaseous AO and solid surface could be efficiently described by the proposed CGMD simulated. According to the reaction criteria, surface recession and heat transfer was also analysed. The CG MD model developed in this research is helpful to study the pyrolysis of polymer networks at larger scales to reduce the gap between simulation and experiment of these complex processes.

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Reactive molecular dynamics simulation study on thermo-resistant properties of thermal protective nanocomposites

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Key Words: *Reactive molecular dynamics simulation, Pyrolysis, Thermal protective nano composites, Activation energy*

In this study, thermo-resistant properties of polyimide and polyimide/inorganic nano particulate composites are investigated by reactive molecular dynamics (ReaxFF MD) simulations. Thermal protective polyimide (TPI) and polyimide-based thermal protective nanocomposites (TPN) used for satellites and ballistic missiles undergo pyrolysis and ablation in ultra-high temperature environment, effectively blocking the heat transferred to the nose cone and fuselage. The most representative method to evaluate the thermo-resistant properties of TPI and TPN is to determine the activation energy by applying the relationship of temperature-reaction rate constant to the Arrhenius equation. In this study, to obtain the activation energy of TPI and TPN, ReaxFF MD simulations were executed under various temperature conditions, and then the relationship of reaction time-thermal decomposition was handled. In order to establish reaction time-to-thermal decomposition relationship of TPI and TPN, two different post-processing methods were used to define the rate constant of the pyrolysis: number of undecomposed chain-based and mass loss-based approaches. The activation energies determined from the two different pyrolysis criteria were compared with each other. In addition, to characterize the properties of soot produced after the pyrolysis, uniaxial tension simulations of carbon network structures remaining after the thermal decomposition simulations were performed. Due to the carbon network structure, the soot layer has very high stiffness compared with unreacted neat polyimide. To validate the activation energy-based thermal resistant property evaluation method, AO (Atomic Oxygen) bombardment simulations were implemented to mimic the in-flight ablation of the TPN. The erosion yield and temperature rising rate of the nanocomposites determined from AO bombardment simulations were qualitatively compared with the activation energy of each nanocomposites structures.

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Temporal homogenization formulation for viscoelastic-viscoplastic materials subjected to local cyclic loading

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Key Words: *Temporal Homogenization; Multiscale modeling; Viscoelastic; Viscoplastic; Cyclic loading*

In this study, the temporal homogenization formulation is developed to predict the response field (e.g., stress, strain, displacement) of the viscoelastic-viscoplastic materials subjected to locally periodic loading. This study is first attempt to apply the temporal homogenization formulation of higher order differential form of the constitutive equation on the viscoelastic-viscoplastic materials. The temporal homogenization formulation is defined two types: the non-updated temporal homogenization formulation and the updated temporal homogenization formulation. In conclusion, the initial boundary value problems are divided into macro-, micro-chronological term. For the verification of this approach, there are two examples: (i) uniaxial cyclic loading on one-dimensional bar, (ii) multiaxial cyclic loading on three-dimensional bar. Comparing the accuracy of the non-updated temporal homogenization formulation and the updated temporal homogenization formulation, it can be clearly seen that the updated temporal homogenization formulation obtained more accurate results.

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Viscoelastic and Damping Characteristics of Boron Nitride Nanotube/Polymer Nanocomposites Including Interface Effects

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Key Words: *Boron Nitride, Molecular Dynamics Simulation, Viscoelastic, Damping coefficient, Quality Factor, Interface*

In this study, molecular dynamics (MD) simulations approach to predict the viscoelastic behavior of boron nitride nanotube (BNNT) polymer nanocomposites is demonstrated. In order to characterize damping coefficient of BNNT polymer nanocomposites, a repeated cyclic loading is applied to the periodic unit cell structure. During the wiggling test, the stored energy and dissipated energy were monitored to determine the quality factor (Q factor) and damping ratio. Some structural defects such as mono- and di-vacancy are considered to understand how imperfections in BNNT affects the interface characteristics and the resultant damping coefficient. At the same time, viscoelastic moduli of nanocomposites were determined from sinusoidal variation of the applied strain and the resultant stress. During the wiggling test, the storage modulus and loss modulus were determined from phase lag between stress and strain which occurs from internal damping. The results show that the Q factor decreases with increasing the driving angular frequency. As the number of defect increases, the damping characteristics and the viscoelastic moduli of nanocomposites were affected by the interface condition as well as the decrease of BNNT's properties in a complicated manner. The possibility of defect engineering to tailor the viscoelastic damping characteristics of BNNT polymer nanocomposites was also discussed.

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A 3D Positivity-preserving and Conservative Multi-moment Transport Model on the Cubed-sphere Grid

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Key Words: 3D global transport model, cubed-sphere grid, multi-moment method, semi-Lagrangian method, mass conservation, positive definite

A three dimensional positivity-preserving and conservative multi-moment transport problem on the cubed-sphere grid was proposed. The numerical solution was calculated by using the dimensional splitting technology to update the horizontal and vertical direction separately. The horizontal direction was updated by the three-point high order multi-moment finite volume method with boundary gradient switching technology, and the vertical direction was updated by the conservative multi-moment semi-Lagrangian (SL) method with the piecewise rational function as spatial reconstruction profile. Some corrections were also involved to ensure a positive numerical result. To evaluate the performance of the proposed model, the transport test cases in the Dynamical Core Model Intercomparison Project were conducted. The numerical test results showed that the model was inherently conservative, non-oscillatory and positivity-preserving. Compared with other existing models in the literature, the proposed model was quite competitive. Furthermore, the semi-Lagrangian method in vertical direction can effcetively avoid the CFL restriction problem caused by the dense vertical grid mesh in real atmopsheric model, which is attractive for practical application in full weather or climate model.

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A High-Fidelity Physics-Based Approach for Space Weather Modeling

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Key Words: space weather, physics-based model, high-order discontinuous Galerkin, GPU

Empirical models of the Earth's atmosphere have been traditionally used to understand the system response to different space weather events based on observational data [1]. However, their limited forecasting capability, specially given the sparse data availability, has prompted in recent years the development of a number of physics-based models, such as the global ionosphere-thermosphere model (GITM) [2], which offer improved prediction capabilities. Their advanced modeling properties, though, come at a high computational cost: solving nonlinear and very high-dimensional systems of conservation laws over long intervals of time.

For this reason, this work presents a high-fidelity physics-based approach for the simulation of space weather on graphic processors (GPUs). The proposed model of the Earth's ionosphere-thermosphere describes an atmosphere in non-hydrostatic equilibrium, driven by the external excitation of solar extreme ultraviolet (EUV) radiation. The conservation equations of continuity, momentum and energy are equipped with realistic data-driven source terms to model heat transfer effects. Moreover, the multiscale variations of the different physical quantities in the radial and angular directions are managed in a fully coupled description, introducing a proper scaling to the momentum and energy variables, and the logarithm of the density as a primary variable to handle the low densities present at high altitudes.

The system is solved using a high-order implicit discontinuous Galerkin (DG) method on unstructured adapted meshes combined with diagonally implicit Runge-Kutta (DIRK) schemes. The numerical discretization is combined with a Jacobian-free Newton-Krylov strategy and matrix-free preconditioners suited to perform on GPU architectures [3, 4]. The proposed method is validated by means of a series of numerical benchmarks and compared to existing reference solutions.

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A Hybrid Volume of Fluid and Level Set Interface Capturing Scheme with Quartic Surface Representation for Unstructured Meshes

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Key Words: Moving interface, Quartic surface polynomial, Volume of fluid, Level set, THINC, Unstructured meshes

In this paper, we developed a hybrid volume of fluid (VOF) and level set interface capturing scheme with quartic surface representation for unstructured meshes. The so-called THINC-scaling scheme with quartic surface representation (THINC-scaling/QSR) preserves the merits of the mass/volume conservativeness from the VOF scheme along with the geometric faithfulness from the level set scheme. Compared with linear/quadratic surface representation used in many other interface capturing schemes, the fluid interface is defined more precisely as a quartic polynomial surface of THINC function which synchronize the interface between the VOF and level set function in a straightforward solution procedure. We update the VOF function using a finite volume formulation. The level set function is first locally updated via a semi-Lagrangian method for interface cells and then reinitialized within each time step. Multi-dimensional algorithm has been developed and verified by some benchmark tests on unstructured meshes. Convincing evidence suggests that the present scheme, with quartic surface representation, can provide high-fidelity solution with more pronounced sub-grid interface capturing capability than other most advanced methods.

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A moist nonhydrostatic atmospheric model by multi-moment constrained finite volume method

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Key Words: *multi-moment scheme, tracer advection, nonhydrostatic model*

A moist nonhydrostaic atmospheric model is developed by using a 3-point multimoment constrained finite-volume (MCV) method. The MCV scheme is local reconstructed scheme like DG and spectral element schemes and can achieve high accuracy. The model variables are the pointwise values of the physical fields located at the equidistant solution points. The constraint on the volume-integrated average (VIA) rigorously guarantees the numerical conservation. The tracer advection is key process for transporting the vapor and precipitation in the real atmosphere. To suppress the unphysical noises for tracers, the non-oscillatory limiter has been adopted in the present model. The resulting model is validated by a well-established benchmark test and compared with the existing compressible model.

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A Non-Negativity Preserving Transport Model Using Multi-Moment Finite-Volume Method and Icosahedral-hexagonal Grid

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Key Words: *Non-negativity Scheme, Multi-moment Method, Transport Model, Icosahedral-hexagonal Grid*

A global transport model with non-negativity property was developed by implementing the high order multi-moment finite volume method [1] on icosahedral-hexagonal grid. Our previous studies have shown that the transport model on icosahedral-hexagonal grid has rigorous numerical conservation and third-order accuracy [2], however, the non-negative numerical solution is not guaranteed and nonphysical undershoots are existed in the numerical results, which violates the physical principle.

Two kinds of moments, including the volume-integrated average (VIA) and the point values (PV), are adopted in the multi-moment scheme and this study is focused on assuring the non-negativity of the VIA moment. The negative solutions of PV moments can be directly removed with destroying the numerical conservation. As the spatial discretization of the VIA is accomplished by evaluating the numerical fluxes along the cell edges, a upper limit on the mass leaving the cell, which is found following the basic idea of the Flux-Corrected-Transport (FCT) method [3] proposed by Smolarkiewicz in 1989 , is adopted to impose the restriction on the numerical fluxes. In one dimensional case, the FCT scheme can be straightforwardly applied by revising the values of PV moments defined at cell interfaces. In multi-dimensional case, the numerical fluxes across the cell edges are determined by more than one PVs and each PV defined at cell vertices are involved in calculations of two numerical fluxes in our multi-moment model[4]. As a result, a new flux correction algorithm was designed on two-dimensional icosahedral-hexagonal grid to develop a global non-negative multi-moment transport model.

The proposed non-negative numerical scheme on icosahedral-hexagonal grid is validated by widely used benchmark tests and the numerical results reveal that the non-negativity of the numerical solutions is guaranteed while the high-order accuracy is preserved. The proposed model provides a promising and practical framework for further development of three-dimensional transport models for dynamical cores on icosahedral-hexagonal grids.

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A Nonhydrostatic Dynamical Core of Atmospheric General Circulation Model Using Multi-moment Method on Cubed-sphere Grid

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Key Words: *Multi-moment method, Dynamical core, Nonhydrostatic model, Global model, cubed-sphere grid.*

As one of key components of the atmospheric genernal circulation models, the dynamical core solves the Navier-Stokes equations on a rotating sphere. To construct the high-resolution numerical models for weather and climate predication, great efforts have been paid recently to improve the dynamcial core, mainly considering its mesh quality, discretization accuracy, computational efficiency, model rebustness and so on.

A nonhydrostatic dynamical core has been developed by using the multi-moment finite volume method that ensures the rigorous numerical conservation in this study. To represent the spherical geometry free of polar problems, the cubed-sphere grid is adopted. A fourth-order multi-moment discretization formulation [1] is applied to the nonhydrostatic governing equations cast in local curvilinear coordinates on each patch of cubed sphere through a gnomonic projection. In vertical direction, the height-based terrain-following grid is used to represent the topography. To get rid of the CFL stability restriction imposed by relatively small grid spacing in the vertical direction, the dimensional-splitting time integration using the HEVI (Horizontal Explicit and Vertical Implicit) strategy is implemented by applying the IMEX Runge-Kutta scheme.

The proposed dynamical core has been extensively verified by the widely-used benchmark tests [2] in comparison with other existing dynamical cores. The results of our numerical experiments show that the present numerical framework has superior solution quality and great practical potential as a platform for atmospheric models. A new unified model for numerical weather prediction and global atmospheric circulation simulation based on this dynamical core is under development in CMA.

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A Versatile OpenFOAM Solver for High-fidelity Simulation of Incompressible Multiphase Flows based on THINC Scheme

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Key Words: Multi-phase flow, THINC/QQ, VOF, Interface capturing, AMR, Supercavitation

Numerical simulations of multi-phase flows involving immiscible interfaces are an active research topic with great importance in a wide variety of environmental, industrial and engineering applications. However, the numerical modeling of interfacial multi-phase flows is fraught with challenges that are inherently complicated in handling the topologically changing interfaces between the two phases, particularly for the unstructured grids. In this talk, we revisit to THINC/QQ (Tangent of Hyperbola INterface Capturing methods with Quadratic surface representation and Gaussian Quadrature)[1] and presents some recent progresses made extensively to improve numerical accuracy and robustness. Then, we develop accurate and efficient solvers for interfacial multi-phase flows based on the framework of OpenFOAM by combining it with PISO (Pressure Implicit with Splitting of Operators) algorithm, as well as AMR (Adaptive Meshes Refinement) techniques. Furthermore, we also develop high-fidelity numerical solvers for turbulent cavitation flows based on the homogeneous equilibrium model. The so-called thincFoam is versatile and potent, offering sufficiently high accuracy for practical applications.

Two and three-dimensional benchmark tests are carried out by solving VOF advection equation on different type of grids. It is convinced that the proposed THINC/QQ scheme shows superior numerical accuracy, robustness and boundedness than original one, and is competitive to the other state-of-art VOF methods. We present some numerical examples such as dam break, bubble rising and RT instability to evaluate the performance of multiphase solver. The numerical results are in excellent agreement with the experimental data and analytical solutions, and show significant improvements in solution accuracy and computational efficiency compared with those of interFoam. Additionally, supercavitation simulations are carried out around an axisymmetric projectile and a conical cavitator at different cavitation number. Our results demonstrate much less numerical sensitivity and solution dependency on the different choice of turbulence and mass transfer models. We believe that the present solvers will be one of the attractive choices in the high-fidelity simulations of multiphase flows involving complex geometries.

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An Adaptive Global Nonhydrostatic Atmospheric Dynamical Core on Cubed Sphere Using Multi-Moment Constrained Finite Volume Method

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Key Words: *Adaptive Mesh Refinement, Nonhydrostatic Atmospheric Model, Dynamical Core, Multi-Moment Constrained Finite-Volume Scheme*

An adaptive 3D global nonhydrostatic dynamical core is proposed on cubed-sphere grid, using the multi-moment constrained finite-volume (MCV) scheme [1] and the Berger-Oliger adaptive mesh refinement (AMR) algorithm [2]. As a newly developed high-order method, the MCV scheme is featured by compact reconstruction stencil and rigorous numerical conservation constrained by the updating of the volume-integrated average (VIA) moment.

The AMR grid of Berger-Oliger includes several groups of grids with different resolutions. During a simulation, refined grids are generated adaptively according to the structure of flow field. Each grid is defined independently and it can be discretized and integrated directly by the same MCV scheme. This makes the extension to the cubed-sphere grid easier as the curvilinear coordinates on each patch of the cubed-sphere are structured. Efforts are mainly spent on the designs of numerical formulations for the coarse-fine interpolation and the flux correction for properly exchanging the solution information among grids of different levels and patches. Considering the fact that the global atmospheric dynamics is mostly dominated by horizontal motions, AMR procedure is only applied in horizontal directions in this study, though no technical problem in generalizing it to a 3D case exist. To avoid impractical small time step restricted by the very large ratio between the horizontal and the vertical grid spacing, the implicit-explicit (IMEX) Runge-Kutta method [3] is introduced as time-marching scheme. The vertical-related terms are advanced by implicit time integration and available time step will be determined only by stability condition in the horizontal directions.

Typical benchmark tests with topography are carried out to evaluate the proposed model. The numerical results on uniform and AMR grids reveal the effectiveness of the AMR technique in saving computational costs, and the accuracy on uniform grid is largely maintained when adaptive grids are implemented. More and more attention being paid to the finer predictions of small-scale weather phenomena has led to a huge demand for computing resources. Using AMR grids, these spatially complex small-scale phenomena are fully described with as few computing resources as possible, thus it is promising to develop an efficient practical atmospheric core under the proposed adaptive framework.

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Development of a Numerical Scheme in Computational Fluid Dynamics Based on a Mesh-Constrained Discrete Points Formulation

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Key Words: *Discretization, Mesh constraint, Moving least squares, Continuum fluid dynamics, Large-scale parallelization*

ABSTRACT

A meshfree/meshless method is a powerful computational tool in continuum mechanics in various physics, engineering, and biological problems. Especially, the methods based on a strong formulation are practically useful that is a complete mesh free [1]. However, in general, the meshless methods tend to be computationally expensive compared to mesh/grid-based methods. That arises from increasing the computational cost to find neighboring calculation/discretization points in gradient calculations using randomly distributed configuration even if applying background meshes (or buckets) approach. In addition, for an implementation to parallel computing with domain decomposition, it is necessary to make a large effort to maintain the computation load per parallelization node evenly. Moreover, in the meshfree methods based on a Lagrangian description (e.g., [2]), the discrete point positions are updated in every timestep and frequently update bucket information with non-uniform internode communication. Therefore, the development of more practical and efficient meshless methods promises to be useful in large-scale simulations.

In this study, we develop a novel discretization scheme for continuum analyses using a mesh-constrained discretization point formulation that becomes a hybrid approach using the meshless and mesh-based ideas. In the present method, discrete points are introduced in background meshes and re-distributed so as to fit arbitrary boundary shapes, where the points are completely confined in (or constrained by) each corresponding background mesh. This allows to efficiently calculate spatial gradients using the MLS approximation [3] and capability in high efficiency in large-scale parallel computation. The method was validated through a numerical example for the two-dimensional Taylor-Couette flow.

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Development of Isolated Element Method and Analysis of Upper and Lower bound solutions by a New Mixed-Hybrid Variational principle

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Key Words: *Isolated element method, Node-less element, Variational principle, Rigid body displacement, Upper and lower bounds, Finite element method*

A new discretization analysis method named the isolated element method [1], that differ from conventional FEM, for solid mechanical problems is proposed. An object to be analyzed is divided into the elements that are separated from each other. A set of displacement functions providing arbitrary number of degrees of freedom is used for each isolated element which expresses the translation and rotation of a rigid body. The extended principle of minimum potential energy is applied to satisfy the continuity of the displacement of isolated elements adjoining to each other. Any node or spring, penalty functions and Lagrange multipliers are not used in this method. The displacement functions of the power series are used to describe the mechanical state of the isolated element and finally, the coefficients of series are determined by a variational principle derived from the extended principle of minimum potential energy.

Furthermore, a new mixed and hybrid variational principle [2] which is composed from the potential and the complemental energy functional is proposed. The pair of these energy are constrained by a formula. Using this new principle, in which stress and displacement can be used as independent variables, the stress and displacement are computed at the same time. Besides, upper and lower bounds solutions are analyzed using the new principle and the isolated element method.

Some computed examples of the plane stress problems are presented. We show the good convergency of the numerical results, and also present the upper and lower bound results of stress and displacement by the new mixed and hybrid variational principle using the isolated element method

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High-fidelity BVD Schemes on Hybrid Unstructured Grids for Single and Multi-phase Compressible Flows

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Key Words: Compressible folws, Discontinuities, Low-dissipation, BVD schemes, Unstructured grids

Compressible flows containing both discontinious and smooth structures are widely encountered in practical problems, such as aerospace engineering, internal combustion engine, energy and chemical industries, to name but a few. It still remains a great challenge for finite volume schemes to numerically solving such complex flows on unstructured grids, where implementing low-dissipative limiting procedure to suppress numerical oscillation faces many difficulties. As a result, most of the unstructured finite volume method for compressible flows are constructed based on second-order schemes which are too dissipative to resolve fine structures such as shockes, interfaces and vorticities. In this talk, we propose a novel hybrid scheme to resolve discontinuities and smooth structures on hybrid unstructured grids. Numerical dissipation is reduced by adaptively choosing appropriate reconstruction scheme based on the one-step Boundary Variation Diminishing (BVD) algorithm[1]. As a results, the MUSCL (Monotone Upstream-centered Schemes for Conservation law) scheme with the MLP slope limiter[2] is adopted to solve smooth regions, while the multi-dimensional THINC/QQ scheme[3] is used to mimic the discontinious solution. The so-called MUSCL-THINC/QQ-BVD scheme is algorithmically simple and shows great superiority compared with other existing schemes for compressible flows on unstructured grids. The performance of present scheme has been extensively verified through benchmark tests of single and multi-phase compressible flows.The numerical results show that the proposed solvers developed upon MUSCL-THINC/QQ-BVD scheme are capable of capturing sharp discontinuous profiles without numerical oscillations and resolving vortical structures along shear layers and material interfaces with solution quality superior to other schemes of second and even higher order.

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Large-eddy Simulation of Turbulent Flows over Sphere Based on High-order Schemes

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Key Words: High-order schemes, Turbulent flows, LES, Sub-critical Reynolds numbers

As arguably the most basic three dimensional geometry, the sphere is considered as an excellent prototype for understanding the wake flows of more general bluff bodies in the engineering applications. In the present study, large-eddy simulations are carried out to investigate unsteady flows around a sphere at sub-critical Reynolds numbers (Re, based on the diameter of the sphere and the freestream velocity). In order to sufficiently capture the turbulence structure, we develop a high-fidelity numerical model for incompressible flows on the unstructured grids which is constructed based on implicit discretization of FVMS3 [1] (Finite Volume method based on Merged Stencil with 3rd-order reconstruction) scheme and fraction-step approach for pressure-velocity coupling.

The performance of this model is first verified by the benchmark test of the steady and unsteady laminar flow at Reynolds numbers of up to 300. The results of hydrodynamic forces, local pressures, and near-wake structures computed by the present solver is examined with adequate solution quality compared with experimental records. In addition, A highly organized flow dominated by periodic vortex shedding, the hairpin vortices has been observed at $Re = 300$, also in good agreement with previous work. After validation, for flow around a sphere at $Re = 1 \times 10^4$, the spatial and temporal features of flow structures at different scales were further explored with respect to mesh type (hexahedra, polyhedra, tetrahedra, and prisms). Special attention is devoted to assessing the prediction of the statistical properties of turbulence, such as wall-pressure distribution, skin friction, and drag coefficient, in order to test the present LES closure model. After conducting comparative study, the present numerical framework shows significant improvements in solution accuracy and numerical robustness over conventional second-order schemes. Moreover, coherent structures of turbulent wake and turbulent kinetic energy (TKE) balance, i.e. the production and dissipation of TKE are also investigated to demonstrate the solver's applicability in different and complex mesh topology.

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Particle Filter for Large-Eddy Simulations of Turbulent Boundary-Layer Flow Generation Based on Observations

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Key Words: *Lattice Boltzmann Method, Large-Eddy Simulation, Particle Filter, Adaptive Mesh Refinement*

This paper presents a novel data assimilation method in realistic turbulent boundary layer simulations for the realization of a wind digital twin. We have developed a plume dispersion simulation code named CityLBM based on a lattice Boltzmann method (LBM). CityLBM enables a real time ensemble simulation for several km square area by applying locally mesh-refinement method on GPU supercomputers [1]. We validated CityLBM against plume dispersion experiments in the complex urban environment of Oklahoma City (JU2003, Leach 2005). Mesoscale wind boundary conditions of JU2003 produced by a Weather Research and Forecasting Model (WRF) were given as boundary conditions in CityLBM by using a nudging data assimilation method (Paniconi et al. 2003; Brian et al. 2010). The statistics of the ensemble-averaged concentration values for ~70% of the monitoring data satisfied factor 2 agreements [2].

Although the above validation study was focusing on the expeiments conducted in the morning on July 16, the experiments in the afternoon have been yet to be validated. In the previous study, the coefficient of the nudging data assimilation method, which characterizes the mixture ratio between turbulent flows from the periodic boundary and laminar flows from the WRF data, was optimized for the statistics of turbulent intensity in the morning. However, the same nudging coefficient lead to an overestimation of the turbulence intensity in the afternoon due to atmospheric instability caused by the increased ground temperature. To resolve this issue, we propose a dynamic nudging data assimilation method, where a particle filter optimizes the nudging coefficient based on the observation data. Here, different nudging coefficients are assigned to each ensemble calculation, and are updated to reduce the error of the turbulence intensity between the simulation data and the observation data every 15 minutes. This approach gave reasonable agreements in vertical profiles of the wind speed, the wind direction, and the turbulent intensity compared to the observation data throughout the day, and enabled all-day simulations, where atmospheric conditions change significantly. In this presentation, we will also report the improvement of concentration predictions in the afternoon.

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The application of Piecewise Rational Method in scalar advection of GRAPES

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Keywords: *PRM, scalar advection, GRAPES, semi-lagrangian*

How to better simulate the advection and the distribution of water substance, is of great significance for the improvement of numerical weather prediction, especially for precipitation. The computation of advection process in a semi-lagrangian model requires high accuracy, conservation of mass, positive and preserve of shape. But the QMSL (Quasi-Monotone Semi-Lagrangian) scheme which adopted in GRAPES (Global and Regional Assimilation & Prediction System) suffers a lower accuracy in the strong gradient and discontinuity regional of the scalar field, and cannot be strictly conserved the mass.

This study draws on research progress in the field of computational fluid dynamics, introduce a material advection scheme PRM (Piecewise Rational Method) which based on piecewise continuous rational function into GRAPES, solve the water vapor equation in the flux form, and treat the polar regions with a mix technical. The two advection schemes were compared by a series of stand-alone and in-model ideal test, proofed that compare to QMSL scheme, PRM scheme is of higher precision, especially in the area of large water vapor gradient, the dispersion and dissipation error is smaller, the conservation and shape preserving is also better. Through the examine of batch prediction experiments in GRAPES, verified that the PRM scheme can effectively improve the simulation of the advection and distribution of water substance, promote the effect of precipitation forecast, and also plays a significant role to the enhancement of the comprehensive model performance.

At present, a series of prediction systems based on GRAPES dynamic core adopted this advection algorithm in CMA, including GRAPES_GFS (global, 25km), GRAPES_MESO (China, 10km), GRAPES_MESO_3km (China, 3km), GRAPES_TYM (Indian Ocean and Northwest Pacific, 9km), GRAPES_GEPS (global, 50km), etc.

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An adaptive multiscale finite element method for strain localization analysis with the Cosserat continuum theory

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Key Words: *Multiscale FEM, p-adaptive strategy, h-adaptive strategy, Strain localization, Cosserat continuum, Heterogeneity*

Abstract
Strain localization analysis based on finite element method (FEM) usually requires an intensive computation to capture an accurate shear band and the limit stress, especially in the heterogeneous problems, and thus costs much computational resource and time. This paper proposes an adaptive multiscale FEM (AMsFEM) to improve the computational efficiency of strain localization analysis in heterogeneous solids. In the multiscale analysis, h- and p-adaptive strategies are proposed to update the fine and coarse meshes, respectively. The problem of mesh dependence is handled by the Cosserat continuum theory. In the fine-scale adaptive procedure, triangular elements are taken to discretize the fine-scale domain, and the newest vertex bisection is utilized for refinement based on the gradient of displacement. In the coarse-scale adaptive procedure, a multi-node coarse element technique is considered. By introducing a probability density function for each side of a coarse element, the optimal positions of the newly added coarse nodes can be determined. With the proposed adaptive multiscale procedure, the computational DOFs are reduced smartly and massively. Three representative heterogeneous examples demonstrate that the proposed method can accurately capture shear bands, with an improved computational efficiency and robust convergence.

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Modeling the Amorphous Polymers Behavior from Low to High Strain Rates

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Key Words: *Amorphous Polymers, Constitutive Model, High Strain Rate, Material Parameters Calibration, Multiscale Modeling, Computational Homogenization*

Amorphous polymers find their main application in the military, automotive and aerospace industries where different loading conditions, such as strain rate, temperature, and pressure, are essential. Typically, polycarbonate (PC) and poly(methyl methacrylate) (PMMA) are used in high strain rate applications due to their lightweight and transparency properties, as well as for their toughness and impact resistance. Through the combination of the excellent thermal and mechanical properties of PC and impact properties of ABS, the rubber toughened ternary blend PC/ABS is one of the most successful commercial polymer blends. The understanding of their multiscale behavior is fundamental for developing new products and enhanced materials, capable of responding to the ever-increasing industrial demand.

The intrinsic behavior of amorphous polymers is known to be extremely sensitive to both temperature and strain rate. While an increase in strain rate promotes an increase of stress, an increase in temperature has the opposite effect. Based on experimental results over a wide range of temperatures and strain rates, Bauwens-Crowet [1] observed that the stress increase is more prominent at higher strain rates (or lower temperatures) than it is at lower strain rates (or more elevated temperatures). This phenomenon has been attributed to the activation of a particular molecular mobility, called the β-transition [2].

In the present contribution, we extend the modified Eindhoven Glassy Polymer (EGP) model proposed by Mirkhalaf et al. [3] to predict the thermomechanical behavior of glassy polymers throughout a wide range of strain rates. The predictive capability of the extended model is assessed by comparing its numerical response with experimental data and different state-of-the-art constitutive models for PC and PMMA, and different loading conditions. In addition, the homogenized thermomechanical behavior of the PC/ABS polymer blend at high strain rates is inferred by conducting first-order hierarchical multiscale analyses based on computational homogenization. State-of-the-art optimization algorithms are explored to speed up the identification of the model's material parameters.

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Multi-scale Modelling of TRIP Alloys and Validation with Automated Parameter Identification

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Key Words: Transformation-induced plasticity, Crystal plasticity, Multi-scale, Parameter identification

The combination of high strength and ductility in metals has been pursued in the last decades, leading to the development of steels such as TRIP (transformation induced plasticity). Modelling the macroscopic response of such materials requires the delicate handling of several complex microscopic phenomena, namely slip plasticity and austenite-to-martensite mechanical transformations. Multi-scale models are well-suited for capturing this interplay of mechanisms by directly modelling the microscopic response of each constituent within a polycrystalline Representative Volume Element (RVE).

A fully implicit constitutive model for austenite-to-martensite transformation with coupled austenite slip plasticity, phase transformation and martensite slip plasticity is used in this work [1]. The generalisation of Patel and Cohen's energy-based criterion introduces the effect of mechanically-induced martensitic transformation, coupled with a volume-preserving exponential mapping integrator for slip plasticity in both austenitic and martensitic phases. A rate-dependent regularisation is employed and several numerical techniques are explored to improve the robustness and efficiency in the rate-independent limit.

Parameter identification is a critical step in model validation. Some parameters are related to physical quantities that can be measured, while others can only be found by trial and error. This work describes a method for automatic parameter identification for macro, micro and constitutive responses using multi-objective derivative-free optimisation methods. With this tool, the accuracy and validity of the proposed constitutive model is studied, using experimental and numerical results in the literature (for instance [3]).

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Size Effects in Fully Second-Order Computational Homogenisation

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Key Words: Multi-Scale, Second-Order Computational Homogenisation, Finite Element Method, Size Effects

Multi-scale models based on fully second-order computational homogenisation [1, 2], where second gradient continuum is considered at both the macro and micro-scales, are able to capture size effects due to the micro-constituents. This fact arises from the length scale parameter introduced by considering second gradient constitutive modelling at the micro-scale. This contrasts with standard second-order homogenisation [3], where size effects are only related to the length of the Representative Volume Element (RVE).

In the present contribution, a fully second-order computational homogenisation model at finite strains is presented. Mixed finite elements are employed at both scales to deal with the C^1 continuity requirement. The Method of Multi-Scale Virtual Power is followed to develop the multi-scale formulation in a variationally consistent fashion and Lagrange multipliers are introduced to enforce the boundary conditions on the RVE. An efficient strategy is devised to compute the macroscopic tangents required for coupled-scale FE^2 simulations. Numerical FE^2 experiments of a boundary shear layer are employed to assess size effects introduced by this kind of multi-scale formulation, due to both the RVE length and the micro-constituents' length scale parameter.

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A Numerical Stress-strain Evaluation of Large Intestine Cancer under Stent Treatment

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Key Words: *Large Intestine, Stent Treatment, Finite element method*

A stent is used to treat obstructive colorectal cancer. A stent is a mesh- or tube-shaped medical device made of shape memory alloy. If the stent deployment force is not appropriate, complications such as perforation of the colon and stent dislodgement may occur. In addition, it has been suggested that excessive deployment force in the colon may accelerate cancer metastasis. Therefore, for the development of safer colonic stents, it is important to evaluate not only the deployment force of the stent but also the stress-strain distribution in the cancer and healthy large intestine during stent deployment. However, it is not possible to directly measure the stress and strain distribution in the cancer and the intestine.

The purpose of this study is numerical stress-strain evaluation of the intestine cancer under stent treatment using a finite element method. This paper will present the following topics:

- Material modelling of healthy and cancerous part of large intestine
- Determination of element discretization conditions for high-precision finite element analysis
- Numerical experiments to predict stress and strain distributions under stent treatment with several heights and hardnesses cancers

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Biomechanical Evaluation of the Healed Acetabulum with Fixation System Using Finite Element Analysis: A Case Study

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Abstract: Objective: To analyse the biomechanical characteristics of acetabular internal fixation system for the treatment of complex acetabular fractures and evaluate its effect, and to explore the relationship between internal fixation and the healed bone, so as to provide guidance and theoretical basis for the accurate treatment of acetabular fractures. **Methods:** Based on the CT scan data of the pelvis of a patient cured by acetabular internal fixation system, a healed pelvic model with internal fixators was established by three-dimensional reconstruction technique, and the spring element was used to simulate the main ligaments of the pelvis, and the finite element analysis was carried out under the load condition of gait phase. Through the relevant mechanical indexes such as displacement and stress, the stability of the pelvis and the stress diversion between the acetabulum and the internal fixators were analysed, and the strain energy distribution of the acetabular three columns was analysed according to the acetabular three-column theory. **Results:** Under the combined condition of gait cycle, the displacement of the left acetabulum and the right acetabulum are small, and the stress distribution is similar to that of the normal acetabulum, and the average stress difference between the internal fixation system and the bone is within a certain range. In the whole gait cycle, the strain energy of the central column of the acetabular three-column is relatively large in the support phase, while the strain energy ratio of the anterior column and posterior column of the acetabular three-column increases in the swing phase. **Conclusion:** The acetabular internal fixation system designed according to the anatomical characteristics of the acetabulum and the acetabular three-column theory not only provides effective mechanical support for the good reduction and stable fixation of the fracture, but also conforms to the natural force flow of the bone. the internal fixators are integrated into the normal physiological stress conduction of the pelvis.
Key Words: *Acetabular Fracture, Internal Fixation System, Three-column, Force Flow*

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Computational Hemodynamic Studies of Porcine Pulmonary Artery for Acute Respiratory Distress Syndrome

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Key Words: ARDS, Pulmonary hypertension, CFD, CNN (Convolutional neural network), Covid-19

The clinical definition of ARDS in adults is "Rapid onset of noncardiogenic pulmonary edema", which is an abnormal accumulation of fluid in the extravascular compartments of the lungs. The hemodynamic instability is a primary factor influencing mortality and the mortality rate among COVID-19 ARDS ventilated patients is one of the most disheartening published results in 2020. The important question is, can we correlate flow alterations and ARDS and come up with the good predictors.

The purpose of this study is to characterize flow patterns and several other hemodynamic parameters (WSS, OSI, Helicity) using computational fluid dynamics model by combining imaging data from 4D-Flow MRI with hemodynamic pressure and flow waveforms from control and hypertensive subjects (related to acute respiratory distress syndrome).

A realistic and automated segmented geometry of pulmonary artery for mechanically ventilated conditions (Baseline, ARDS, Optimal Lung Approach, Hyperinflation and Collapse) is obtained by training a (2D convolutional neural network) (CNN) on CTA scans obtained by translating MRA images. Fluid dynamics equations are solved for the subject specific pulmonary arterial meshes. This work considers the utility of computational models in providing insights into identifying abnormal flow features of the pulmonary circulation, and their application in clinically motivated studies related to ARDS.

Specific attention is devoted to mutual validation of quantitative parameters generated from CFD and PC-MRI images. So far, the analysis is done on six subject with five ventilatory conditions(Basal, ARDS, OLA, HI, COL). Different hemodynamic parameters are analysed after in-vivo validation of velocity profiles and then important predictors is presented after statistical validation. This work mainly concerns how to facilitate bench-bedside approach using CFD tools and is a continuation of our previous work with diseased cases.

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Insight of biomechanical implications on membrane infolding in the covered stent - from computational and experimental perspective

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Key Words: *Finite element analysis (FEA); Computational fluid dynamics (CFD); Carotid artery stenting (CAS); Nitinol; Stent; Membrane; Covered Stent; Infolding*

Carotid endarterectomy (CEA) is the gold standard preventative treatment for high-grade carotid artery stenosis. However, CEA is invasive and often associated with a higher risk of ipsilateral stroke and death. Recently carotid artery stenting (CAS) has emerged as an attractive alternative due to its less invasive procedure that can help to prevent stroke in patients with carotid artery stenosis. But stenting using bare-metal stent is poor in preventing the detached plaque into cereal circulation. A covered stent can provide better protection to avoid thrombosis. However, the conventional dip-coating method may trigger the membrane infolding in the covered stent that was found to affect the mechanical performance of the covered stent in the artery.

To minimize the effect of membrane infolding, we have proposed a new coating method by pre-crimping the covered stent before coating. Detailed structural analyses were performed on the conventional dip-coating method and the proposed new method. A multi-step simulation was performed on the covered stent to evaluate the stress distribution across the covered stent. In addition, we also investigated the hemodynamic behaviour of the covered stent using computational fluid dynamics (CFD) to evaluate the risk of thrombosis after deployment. Non-Newtonian fluid model and realistic boundary conditions were used in the current study to model the realistic blood flow behaviour.

The higher von Mises stress was found in the membrane of the covered stent manufactured by the conventional dip-coating method after infolding occurred, compared to the new method in the structural mechanics analysis. Our new pre-crimped coating method minimised the deformation as examined in our computational study, followed by experimental testing. CFD results showed that our new pre-crimped covered stent could reduce the risk of thrombosis compared to the conventional coating method. No platelet activation was found in the animal experiment using our pre-crimped covered stent compared to the conventional dip-coating method. Both computational and experimental results showed satisfactory mechanical performance in mitigating infolding of covered stent.

In conclusion, our study showed that our new coating method is better than the conventional dip-coating method for reducing membrane infolding in the covered stent and may reduce the risk of thrombosis after its deployment.

Time-dependent topology optimization and machine learning modelling for tissue scaffolds considering bone ingrowth

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Key Words: *Topology optimization, Machine learning, Scaffold, Bone ingrowth, Modelling*

Large bone defects caused by diseases, trauma and injuries remain a challenging healthcare issue. The treatment by synthetic tissue scaffolds have gained substantial attention from research and clinical communities attributable to their potential to overcome risks of infection, diseases transmission, donor site morbidity and tissue shortage associated with conventional treatments. In bone tissue engineering, the structural characteristics of scaffolds on-site play an important role in their biomechanical properties that notably affect the outcome of physical loading/mechanical stimulus regulating neo-bone formation in scaffolds. Compared to time-consuming and expensive trial-and-error experiments, computational modelling techniques have been in favour for the investigation of bone scaffolds for their compelling efficiency and strong predictive features. For bone-scaffold construct system, bone ingrowth and scaffold degradation lead to continuous variations of mechanical stimulus in a time-dependent fashion. On the one hand, such dynamic nature in bone-scaffold construct system requires for time-dependent optimization design of bone scaffolds. On the other hand, the dynamic nature renders computationally efficient issues for modelling bone ingrowth, especially for bulk scaffolds whose computational cost is prohibitive by using conventional finite element (FE) method. To address these challenging issues, we proposed a time-dependent mechanobiology-based topology optimization framework for design of bone scaffolds by considering an ongoing favourable microenvironment ensuring a long-term outcome for bone regeneration, in which a level-set based topology optimization algorithm and a time-dependent shape derivative were developed to optimize the scaffold architecture [1]. We also proposed a machine-learning (ML) based multiscale model to predict bone ingrowth outcomes in bulk scaffolds, in which the microscopic modelling was fully implemented by ML and significantly reduced the computational cost into a significantly efficient level [2]. The proposed approaches pave a new avenue for computational design and modelling of bone scaffolds, which are expected to form a promising tool for future studies by taking into the consideration of bone ingrowth outcome in scaffolds.

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Energy stable moving mesh strategy for simulating dynamics of millimetric droplets on inclined non–homogeneous surfaces

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Key Words: finite element method, moving mesh, arbitrary Lagrangian–Eulerian, generalized Navier boundary condition, energy stability

In this work we develop a numerical model for simulating the dynamics of millimetric droplets on inclined and non–homogeneous surfaces. Such scenarios may exhibit various regimes of different complexities such as droplet spreading, sliding and rolling. Study of droplet behaviors under different conditions attracts more and more attention due to (potential) industrial applications in microfluidic related areas. We employ *finite element method* (FEM) within *arbitrary Lagrangian–Eulerian* (ALE) framework. Under the (reasonable) assumption that there is no topology change in the droplet shape, ALE framework is a natural choice due to its ability to capture the flow dynamics and credibly track the free surface.

Stability of the numerical scheme in energy norm is (relatively) easy to satisfy on stationary meshes while it becomes non–trivial and challenging task for discretization on moving meshes. Energy stability is desirable property since it guarantees that time discretization does not introduce spurious energy into the fluid system. The main goal of this work is the development of an energy stable moving mesh strategy within ALE FEM model. The essential ingredients are the so called *space conservation law* (SCL) (see [1]) and employment of Laplace–Beltrami operator for the interface curvature evaluation (see [2]). Primary aims in designing mesh updating strategy are to keep the good quality of the mesh and to minimize the frequency of re–meshing. Considering that the droplet dynamics can simultaneously exhibit both sliding and rolling regimes, together with the energy stability requirement, such task becomes quite challenging.

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Functional Analysis of Healthy and Heart Failure Tissue Populations using 3D Cardiac Electromechanical Models

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Key Words: *Cardiac biomechanics, Uncertainty quantification, Cardiac disease*

Computer modelling and simulation of the beating heart must reflect on electrical activation of cells and tissue, mechanical properties of tissue, and their interaction. Electrophysiological properties of the heart have been simulated abundantly and applied to increase mechanistic understanding of disease and improve treatment development. Recent maturity in cardiac mechanical modelling increased quantitative predictive power. However, tight coupling of cardiac mechanics with the underlying electrophysiological properties of the tissue makes modelling clinical mechanical phenomena such as cardiac disease and drug effects difficult. A combination of uncertainty quantification through populations of models and fully coupled electromechanics models provide greater predictive power on cardiac mechanisms and aid treatment development for cardiac diseases.

A fully coupled electromechanics model of ventricular tissue is developed by coupling the O'Hara-Rudy[1] electrophysiology model and the Land[2] mechanics model. A population of models was created by varying 16 electrophysiological and 11 mechanical parameters at the cell level. The population was calibrated from 1000 to 187 models based on biomarkers derived from the action potential shape, calcium transient and active tension. This calibrated population was altered in 11 parameters of the cell model to represent heart failure (based on [3]). A geometry of 20x7x3 mm is simulated with 1.0 or 0.5 mm spatial resolution for mechanics or electrophysiology respectively, with free movement in the fibre direction on one side. Results are extracted at the centre of the tissue, as well as tissue shortening on the free-contracting side.

Relative to the healthy population, heart failure manifests in both electrophysiological and mechanics biomarkers. The action potential takes ~20% longer to recover from activation and peak calcium concentration in the cell is reduced by 50.9%. In a similar trend, mechanical biomarkers show 42.2% reduction in peak active force, slower contraction and more variation in recovery times across the heart failure tissue population. The peak tissue shortening in the fibre direction as a result of free contraction is reduced from 0.68±0.07mm to 0.45±0.07mm (-33.2%) and its peak is delayed by 112ms (38.6%) in heart failure.

These simulations indicate strong effects on electrophysiological and mechanical heart function by population variation and disease such as heart failure. Therefore, strongly coupled 3D models are necessary to assess the impact of biological variation, cardiac vulnerability as well as safe and effective treatment development.

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Investigation of the Inertial Cavitation Threshold under a Dual-Frequency Acoustic Signal in Various Soft Tissues

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Key Words: *HIFU, Inertial Cavitation Threshold, Dual-frequency Driving Signal*

High-intensity focused ultrasound (HIFU), it's applications, and accompanying acoustic cavitation have been of great interest in biomedical engineering. HIFU therapy is a non-invasive method for tumor ablation in different organs: prostate cancer, liver, pancreas, breast, kidney, bone and soft tissue tumors [1]. One of the main mechanisms of focused ultrasound ablation is the thermal effect. However, at high ultrasound powers cavitation may appear during the treatment. Cavitation can lead to local temperature enhancement, which can be helpful during the treatment. However, it is quite difficult to control the effects of cavitation. Fundamental understanding is necessary for the further development of the technology.

At low ultrasound pressures, bubbles experience stable oscillations. When pressure reaches some critical threshold value, bubbles start to collapse. Bubble collapse is accompanied by a big increase of the local temperature and correspondingly in larger ablated volume [1]. This type of cavitation is called inertial cavitation which is investigated in the current study. We investigated the inertial cavitation threshold by analysing the dynamics of a single bubble in viscoelastic tissue.

The objective of the present study is the numerical investigation of the inertial cavitation threshold in soft tissue and its dependency on excitation parameters (single- and dual-frequency signals of HIFU), since inertial cavitation can lead to high extreme temperatures, sonoluminescence, and sonochemistry. In order to investigate the inertial cavitation threshold, acoustic wave propagation was modeled by generalized Westervelt equation [1], whereas bubble dynamics was modeled in a viscoelastic tissue by using the Gilmore-Akulichev-Zener model [2]. The inertial cavitation thresholds for different criteria, for different modes of the acoustic signal, and for different initial bubble sizes were computed. A comparison of released energy from different cavitation regimes was made. In addition, the optimal frequency combinations for a dual-frequency signal were found. The impact of different viscoelastic tissue properties and nonlinear acoustic effects on the bubble dynamics, threshold pressure, and optimal frequencies was studied.

The obtaining results demonstrated that a cavitation threshold criterion, based on a bubble size, gives lower threshold values than a criterion using bubble collapse velocity. An increase in the values of viscosity and elasticity leads to a rise in the threshold amplitude. Optimal frequency combination in dual-frequency signal mode can deliver the lowest threshold pressure that will be approximately the same for the different initial bubble sizes. Our study can provide a more detailed understanding of the inertial cavitation process and can also help to control side cavitation effects during HIFU therapy.

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Mathematical modeling of ion transport through an ion channel

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Key Words: Ion channel flow, PNP, non-ionic interactions, ion solvation, LBM-IBM, GPU

Ion transport in the presence of fixed an free charges, in a dielectric medium can be described through Poisson-Nernst-Planck (PNP) equations. PNP equations, account for ionic interactions between ions and assume ions to be volumeless. These assumptions, however, restrict PNP equations to dilute flows. In case of flow with high ionic concentration, confined channel geometry or flows where non-ionic interactions play a significant role, PNP equations must be modified. Ion channel flow is one such system. Several extensions to PNP equations exist based on the requirement of the system. For example, Lennard-Jones model [1, 2] or Bikerman model [3, 4] can be added to PNP equations to account for the effect of non-ionic interactions. Effect of ion solvation can be included by introduction of Born solvation energy model [5, 6] or non-local electrostatics [3, 4]. Typically, in Bikerman model, transport of water molecules as a response to electrostatic and steric potential is included which is typically diffusive in nature. One can further modify these equations by including nonlinearlity and effects of viscosity of the fluid (water)for channels where, in addition to ions, water also permeates. This can be accomplished by coupling modified PNP equations with Navier-Stokes equations. Governing equations are descretized using lattice Boltzmann method. For adequate implementation of boundary conditions, immersed boundary method has been used. Further the code has been parallelized on multiple GPUs using CUDA.

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Numerical Simulation of Coagulation Cascade in Aortic Dissection with Two Tears

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Key Words: *Coagulation cascade, Thrombosis, Aortic dissection, Fibrin, Computational fluid dynamics*

Objectives: Type B aortic dissection (TBAD) is a major aortic catastrophe that can be acutely complicated by rapid expansion, rupture, and malperfusion syndromes. The separation of the intima from aortic walls will form a second blood-filled lumen defined as "false lumen (FL)", where the thrombus is more likely to form due to the local stasis hemodynamic conditions [1]. However, the thrombosis mechanism is still unclear and little is known about the impact of the chemical species transported by blood flow on this process. The proteins involved in the coagulation cascade (CC) may play an important role in the thrombosis process, especially in the activation and stabilization of platelets [2].
Methods: Based on the further development of the model introduced by Anand et al. [3, 4], we established a reduced-order fluid-chemical model to study the CC process in dissected aorta under realistic flow conditions. An idealized three-dimensional TBAD phantom with two tears was adopted to investigate potential thrombosis in FL and study the effect of hemodynamics on this process. The FL wall and the true lumen wall are regarded as "injury wall" and "healthy wall", respectively, and a series of boundary fluxes are set for the injury wall to describe the surface reactions occurring there.
Results: A high level of fibrin is continuously observed at the top of the FL and some time-varying areas between two tears, indicating a high likelihood of thrombus formation there. This finding is consistent with the clinical observation. The time evolution of coagulation factors is greatly affected by local hemodynamics, especially in the high disturbance zone, the evolution has characteristics of periodic changes consistent with the flow field. The ability to reproduce the CC response of the proposed model also provides a potential application to integrate with a model that can simulate platelet activities, forming a biochemical-based model which would help unveil the mechanisms of thrombosis in FL and the clinical decision of appropriate treatment.

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Biomolecular Mechanics Revealed From Gaussian Accelerated Molecular Dynamics

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Key Words: *Gaussian Accelerated Molecular Dynamics (GaMD), G-protein-coupled receptor (GPCR), Allostery, Intramembrane Proteolysis, Drug Discovery.*

Gaussian accelerated molecular dynamics (GaMD) is a robust enhanced sampling technique that works by applying a harmonic boost potential to reduce system energy barriers and accelerate biomolecular simulations by orders of magnitude[1]. Since publication in 2015, GaMD has received 350+ citations in the field. GaMD has been implemented in widely used simulation packages including AMBER, NAMD, OpenMM, GENESIS and Tinker-HP. GaMD has been also combined with compatible methods such as Replica Exchange, Umbrella Sampling, Adaptive Biasing Force and Weighted Ensemble for further improved sampling and free energy calculations. Recent developments of new Ligand GaMD (LiGaMD)[2], Peptide GaMD (Pep-GaMD)[3] and Protein-Protein Interaction GaMD (PPI-GaMD)[4] algorithms have unprecedentedly enabled microsecond atomic simulations to capture repetitive dissociation and binding of small-molecule ligands, highly flexible peptides and proteins, thereby allowing for highly efficient and accurate calculations of their binding free energies and kinetics. In addition to protein folding and conformational changes, ligand binding, protein-protein/membrane/nucleic acid/carbohydrate interactions[1], I will talk about recent applications of GaMD that have revealed dynamic mechanisms of, among others, G-protein-coupled receptor (GPCR) allostery[5] and intramembrane proteolysis by γ-secretase[6-7], and facilitated drug discovery[5].

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Conformational Entropy of FG-Nucleoporins Plays the Key Role in Creating the Selective Transport Barrier in the Nuclear Pore Complex

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Key Words: *Nuclear Pore Complex, FG-Nucleoporin, Intrinsically Disordered Protein*

The nuclear pore complex (NPC) is a protein complex that perforates the nuclear membrane creating the transport channel between the nucleus and the cytoplasm [1]. The NPC is composed of about 30 different proteins called nucleoporins (Nups), each of which having multiple copies in one structure. The Nups located in the central channel region are phenylalanine- and glycine-rich Nups (FG-Nups), which are intrinsically disordered and tethered on the channel wall of the NPC. FG-Nups create the selective barrier against molecular transport through the NPC; while small cargoes (less than 5-9 nm) can pass through the nuclear pore freely, large cargoes can do that only when they are bound to the nuclear transport receptors (NTRs). The selective transport is essential for the cell, but how exactly FG-Nups create such an exquisite barrier remains elusive. In our study, we hypothesized that the change in free energy associated with the conformational freedom of FG-Nups is the critical factor determining the selectivity. When a large cargo is translocating through the nuclear pore, it restricts the space available to FG-Nups decreasing their conformational entropy (and thus, increasing the free energy of the system), which virtually prevents cargo's passages. On the other hand, interactions between FG-Nups and NTRs energetically lower the free energy, allowing them to overcome the entropic barrier. To investigate our hypothesis, we computationally modelled the free energy of the system composed of FG-Nups tethered on NPC's channel [2]. We modelled FG-Nups as Gaussian chains interacting with the potential field around the surface of NTRs (that represents the adsorption to them) and calculated the free energy change while inserting a cargo into the nuclear pore. We found that the free energy change was less than thermal energy for small cargoes less than 6 nm in diameter and it was large enough for large cargoes to prevent their passage. We also found that the energetic interaction between FG-Nups and NTRs effectively lowered the free energy barrier, lowering the size limit of the transportable cargoes. This selective behaviour was affected largely by some physical parameters, such as the flexibility of FG-Nups, the length of FG-Nups, and the diameter of the nuclear pore, suggesting the possibility of the mechanical alternation of the selectivity. To further investigate our hypothesis, we simulated the dynamics of the transported cargoes through FG-Nups using a coarse-grained Brownian dynamics model. The simulation result was consistent with the free energy analysis, suggesting the importance of the conformational flexibility of FG-Nups as a key factor creating the selective barrier.

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Disorder-to-order Transition in Multi-cellular Systems

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Living cells interact with one another, and with their extra cellular matrix. These interactions are chemical and biophysical. Interactions lead to collective behavior between cells - essential for tissue formation, morphogenesis, and tumor growth. We hypothesize that cell-cell interaction depends on the distance between them, and there exists a critical distance beyond which interaction cannot take place. We test the hypothesis by forming free-floating discs of cell-ECM mixture in vitro. We find that above a critical cell density, the discs compact and reach a specific size, independent of density. However, the rate of compaction increases with density. Below a critical cell density, the discs do not compact. High speed imaging and fluorescence microscopy reveal the underlying mechanism of this phase transition. Initially, each cell interacts with the surrounding ECM and generates a strain field, while it migrates in a Brownian motion. In contrast to the conventional view, the cell does not remodel the matrix. It does not cause any permanent deformation. The strain field is transient and reversible. At low cell density (cells are far apart), the cells do not “see” the strain field of any neighbor. They continue their Brownian dynamics without leaving any memory behind. Global symmetry is maintained without any collective behavior. The discs do not compact, independent of cell density. With increasing cell density, the cells come within their neighbors’ strain field. The probability that the two neighbors’ strain field getting aligned, both temporally and specially, increases. This breaks the global symmetry. Cells begin to interact in a feed forward way, forming a network between them, compacting the disc. The final compacted state becomes independent of the initial density. We develop a one-dimensional mathematical model of cell-cell-ECM interactions to explain the observations. The model accounts for time dependent ECM deformations mediated by the cells and their acto-myosin machinery, non-linear viscoelasticity of ECM, and the feedforward compaction process. The model captures the disorder-to-order transition as a function of cell-cell distance.

Effect of hydrostatic pressure on TRV1 conformation using molecular dynamics simulation

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Key Words: *Glaucoma; Hydrostatic pressure; Mechanotransduction, Molecular Mechanics*

Glaucoma is one of the eye diseases where the retinal ganglion cells (RGCs) die, resulting in the loss of eyesight. The most common factor to cause glaucoma is an elevation of intraocular pressure (IOP). However, the mechanism that IOP causes cell death in detail remains unknown. High hydrostatic pressure applied to incubated RGCs increased Ca^{2+} concentration in cells and cell death, though they were suppressed by the antagonist of transient receptor potential vanilloid 1 (TRPV1), a membrane protein [1]. This study strongly suggests that the TRPV1 is the mechano-sensor to respond to hydrostatic pressure, open its channel, and transport Ca^{2+} through the channel. Thus, we investigated the conformation changes of TRPV1, focusing on the channel radius under the elevated hydrostatic pressure using the molecular dynamics (MD) simulation.

The PDF file of the TRPV1 structure (5IRZ) was obtained from the Protein Data Bank. Lost side chains were added with the DeepView software. The protein was embedded in 1-palmitoyl-2-oleoyl phosphatidylcholine lipids using the CHARMM-GUI-web server. The MD simulation was performed using the GROMACS software (v. 2020-3) and CHARMM27 force field. Totally 165,201 atoms of proteins, lipids, ions, and waters were generated. The simulation was performed for 100 ns in the NPT ensemble at 37°C and two pressure levels: the ordinary (12.6 mmHg) and the elevated (27.6 mmHg) pressures.

The radius of gyration at the lower gate at the elevated pressure (4.80 ± 0.08 Å) was slightly, but statistically significantly higher than that at normal pressure (4.74 ± 0.08 Å), indicating larger outwards motions of the lower gate at elevated than normal pressure. The lower gate radius at elevated pressure (0.54 ± 0.14 Å) was slightly, but statistically significantly higher than the radius at normal pressure (0.49 ± 0.14 Å), indicating an increase in the lower gate radius at elevated pressure compared to normal pressure.

These results indicate that the radius of the membrane channel TRPV1 increased under elevated pressure. However, the radius is still smaller than that of the hydrated Ca^{2+}, and we hardly conclude that hydrostatic pressure opens the channel to transport the Ca^{2+}. More extensive MD simulations are needed to provide more insight into the effect of hydrostatic pressure on TRPV1.

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Image-based Simulation Study on Mechanosensing Amplification Mechanism at Osteocyte Processes in Bone Canalicular Space

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Key Words: *Osteocyte, Mechanosensing, Image-based simulation, Computational Biomehcanics*

Osteocytes, mechanosensory cells in bone mineralized matrix, are believed to regulate bone remodeling by sensing the flow-induced mechanical stimuli to their slender cellular processes within a canalicular space [1]. However, it is difficult to experimentally evaluate the flow and local strain of the osteocyte process membrane in vivo. In this study, to discuss the mechanosensing amplification mechanism in bone, we constructed an image-based model of osteocyte process [2], tethered to the canalicular wall, and evaluated the local strain concentration by performing fluid-structure interaction simulation [3].

A high-resolution image-based model of an osteocyte process and a canalicular space was constructed using tomographic image data obtained using ultra-high voltage electron microscopy. Tethering elements (TEs), connecting the osteocyte process membrane and the canalicular wall, were modeled as linear elastic springs and randomly arranged within the space. The lattice Boltzmann method [4] was employed for fluid flow analysis governed by the Brinkman equation, and the finite element method was used for membrane deformation analysis governed by Skalak's constitutive law [5], both of which were coupled using the immersed boundary method [6].

With the flow of interstitial fluid, local strain concentration in the osteocyte process was observed near the TEs with high tension, strongly dependent on the flow direction and the orientation angle. These results suggested that the configuration/alignment of TEs relative to the flow direction is an important factor with significant effect on the local strain concentration in osteocyte process membrane, playing an important role in osteocyte mechanosensing in bone remodeling. Further studies on the nanoscale environments of the bone canalicular space may provide a key to elucidating the mechanism of bone diseases and age-related change in bone remodeling.

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Mechanical Positive Feedback Mediated by Pizeo1 and Integrin Causes Irreversible Cardiac Fibrosis

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Key Words: *Positive Feedback, Integrin, Pizeo1*

ABSTRACT

Cardiovascular diseases, including myocardial infarction (MI), hypertension and atherosclerosis, are accompanied by cardiac fibrosis, which involves permanent activation of cardiac fibroblasts (CFs) during myocardial injury, resulting in excessive deposition of extracellular matrix (ECM), thereby increasing the stiffness of the pathological areas. More and more evidences showed that the matrix stiffness plays an important role in CFs activation and cardiac fibrosis, and several signal transduction factors (such as integrin, force-sensitive ion channels) that directly act on the activation of CFs have been identified. However, the key regulatory network perceiving matrix stiffness to regulate CFs activation is still unknown. Here, we detected significantly increased expressions of integrin β1 and Piezo1 in native fibrotic cardiac tissues. By using mechanically regulated in vitro cell culture models, we found that a stiff matrix induced high expressions of integrin β1 and Piezo1 in CFs, accompanied by enhanced cell activation. Importantly, we first found that a positive-feedback loop (PFL) between integrin β1 and Piezo1 enhanced cardiac fibrosis and lead to an irreversible phenotype with increasing stiffness, indicating that the PFL plays an important role in mediating substrate stiffness-induced CFs activation. Further mechanistic studies revealed that Ca2+ and YAP play important roles in integrin β1-Piezo1 positive feedback mediated fibroblast activation. Considering that this PFL is specific to CFs activation, integrin β1-Piezo1 PFL may be a fibroblast-specific therapeutic target to treat fibrotic diseases.

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Mechanical response of T-cell receptors

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Key Words: Adaptive immunity, T-cell receptor, major histocompatibility complex, molecular dynamics

The αβT-cell receptor (TCRαβ) recognizes 8–10 aa antigenic peptide loaded on the major histocompatibility complex (pMHC) molecule with exquisite sensitivity, with a signal-to-noise ratio of 1 in 10^5. Yet, the equilibrium binding affinity of cognate and non-cognate pMHCs are similar and weak, on the order of micromolar range. Recent experimental findings suggest that application of physiological-level picoNewton forces to the TCRαβ-pMHC complex increases the bond lifetime in ligand-dependent manner. This suggests that TCRαβ-pMHC system exhibits catch bond behavior that mechanically enhances antigen discrimination. We address the atomistic mechanism for the activation of the catch bond by performing all-atom molecular dynamics simulation of TCRαβ-pMHC complexes under picoNewton forces and their variants. By comparing subdomain motion and dynamics of interfacial contacts, we find that the applied load suppresses certain modes of domain motion that have destabilizing effect on the TCRαβ-pMHC interface in the absence of load [1]. The dynamical activation of catch bond also allows for allosteric control of the interface by altering the motion of distal domains. The dynamical mechanism also has implications in other types of T-cell receptors.

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Microtubules' Bends, Cryo-Cool Ribosomes, and Wet Proteins

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Key Words: *Ribosomes, Microtubules, Atomistic Simulations, Solvent Enthalpies and Entropies*

Microtubules provide both mechanical support and, via the kinetochore, mechanical forces to the cell. The filaments can undergo growth/polymerisation and shrinking /depolymerisation phases, driven by GTP hydrolysis. Through non-equilibrium atomistic simulations of entire plus-end microtubule tips we show that the average nucleotide state of the plus-end MT tip determines the heights of energy barriers between tip conformations, such that the post-hydrolysis MT tip is exposed to higher activation energy barriers, which translates into its inability to elongate [1].

Much about the ultra-structure of microtubules ─ as well as of many other biomolecules and biomolecular complexes has been revealed by the recent resolution revolution in cryo-electron microscopy. How much of the ambient temperature ensemble of biomolecules is preserved during shock freezing prior to image acquisition is, however, an unsolved question. In shock cooling atomistic simulations of fully solvated ribosomes at realistic time scales we observed, depending on cooling rates, a marked decrease of structural heterogeneity, which we were able to quantify [2]. The observation that a kinetic two-state model improves the prediction of the decrease in heterogeneity compared to the cooling-rate independent thermodynamic model suggests that kinetic effects do contribute markedly. Small barriers between the states (<10 kJ/mol) are overcome during cooling and do not contribute to the heterogeneity of the structural ensemble obtained by cryo-EM, whereas conformational states separated by barriers above 10 kJ/mol are expected to be trapped during plunge-freezing [2]. Our results will allow one to quantify the heterogeneity of biologically relevant room-temperature ensembles from cryo-EM structures.

In these processes, as well as quite generally in protein folding and the thermodynamics of biomolecular stability, the solvent shell plays a pivotal role as, e.g., the effect of cold denaturation clearly demonstrates. We will present a new method to compute solvent enthalpies and entropies with spatial resolution and thus to quantify the underlying thermodynamic enthalpy/entropy tug-of-war [3]. For the example protein crambin, we quantified the local effects on the solvent free-energy difference at each amino acid and identified strong dependencies of the local enthalpy and entropy on the protein curvature. Remarkably, more than half of the solvent entropy contribution arises from induced water correlations [3].

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The Gating Mechanism of the Mechanosensitive Ion Channel NompC

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Key Words: Mechanosensitive Ion Channel, NompC, Molecular Dynamics, Gating, Ankyrin Repeat

Mechanosensitive ion channels are membrane proteins that can respond to mechanical stimuli to open and conduct ions across cell membranes to trigger downstream signaling. NompC is a crucial mechanosensitive ion channel for the sensation of touch and balance in *Drosophila melanogaster*, representing an ideal model for the study of the tethered mechanosensitive ion channels. Based on the Cryo-EM structure of NompC, we performed molecular dynamics simulations to reveal the atomistic details of the channel gating mechanism. Our results showed that a pushing force from the intracellular region can open the channel, but not a pulling force. The supercoiled ankyrin repeat region acts like a spring with a force constant of $\sim$13 pN/nm, which can transfer forces at a rate of $\sim$1.8 nm/ps to the linker helix domain. A subsequent rotation of the TRP domain, which is next to the linker helix domain, was found to be related to the opening of the channel, and the key residues forming hydrogen bonds along the force convey path were identified. We propose that the push-to-open gating mechanism may enable cells to feel external compression or volume shrinkage, and we speculate that a force transformation from pushing to twisting might be the key to the channel gating.

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A multi-physics model for myocardial perfusion in the human heart

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Key Words: *Cardiac perfusion, Multiphysics Problems, Myocardial blood flow*

Myocardial perfusion is the delivery of blood to the heart muscle, supplied by the coronary circulation. Reduced coronary flow rate, due for example to atherosclerosis, can lead to ischemic cardiopathy and, possibly, to an infarct of the myocardium.

We present a mathematical and numerical model for human cardiac perfusion which accounts for the different length scales of the vessels in the coronary tree. Precisely, a clear scale separation can be noticed between the coronaries laying on the epicardium and the smaller vessels penetrating into the tissue [1]. We adopt a multi-physics approach in which the epicardial vessels are represented with a three-dimensional fluid-dynamics description (Navier-Stokes) whereas the intramural vessels are modeled by means of a multi-compartment porous medium (Darcy's law) [2]. These two models are coupled using interface conditions based on the continuity of mass and momentum. Since the heart is composed by regions perfused by distinct epicardial vessels [3], we partition the myocardial domain in perfusion regions. A suitable calibration procedure is introduced to use patient-specific values for the parameters of the model.

The multi-physics approach was used to reproduce myocardial blood flow (MBF) maps in nine patients (four healthy and five with detected coronary artery disease), showing an excellent agreement between the computed MBF and MBF measured from clinical data [4]. The results of this work proved the accuracy and the reliability of the proposed multi-physics model in reproducing MBF. In this way, we could provide a quantification of the MBF avoiding in principle invasive MBF measurements such as using stress CT. This could be useful for the assessment of the coronary artery disease and for guiding revascularization decisions.

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An Efficient Space-Time Adaptive Numerical Method for Fully Coupled Electromechanical Models of Cardiac Tissue

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Key Words: *Space-Time Adaptivity*, *Multiphysics Problems*, *Computational Cardiology*, *Adaptive Mesh Refinement*, *Multirate Timestepping*

Studying the heart using computational models has gained wide attention over the last decade. A large focus area has been the improvement of coupled electromechanical models and their efficient numerical treatment. Electromechanical models, including biophysically detailed mechanisms for excitation-contraction coupling, mechano-chemical, and mechano-electrical feedback, are important candidates to investigate, for example, the mechanisms underlying arrhythmias in diseased hearts. However, these investigations require simulations of full cardiac cycles at the organ-level, which, despite advances over the last years, remain very expensive from a computational standpoint. In order to improve the performance of fully coupled electromechanical simulations we present a novel, general, space-time adaptive framework using the finite element method and an adaptive Godunov-type operator splitting. Since the required element size and time step length for the electrical subproblem are an order of magnitude smaller than for the mechanical subproblem, we nest the mesh for solving the electrical problem into the mesh for solving the mechanical problem. Further, we utilize adaptive refinement of the electrical mesh to drastically reduce the total computational cost during depolarization, while being able to capture the electrical wavefront with high accuracy. Additional speed-up is gained by using a novel time-adaptive operator splitting scheme [1], where the time steps of the electrical problem are nested into the time step of the mechanical problem, which remains constant. The presented framework also utilizes an augmentation of the local adaptive time stepping by Qu and Garfinkel [2]. Verification and work-precision studies are carried out and a study on a realistic biventricular rabbit model with measured microstructure [3] is presented, suggesting a speed-up of more than an order of magnitude while preserving high accuracy.

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Dynamic Fracture of Skin and Subcutaneous Tissue During Auto-injection

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Key Words: *Dynamic fracture, Nonlinear finite elements, Soft Tissue Mechanics*

Delivery of life-saving drugs through injection to the subcutaneous space has increased rapidly, in part due to the introduction of auto-injector devices [2]. Auto-injectors are a convenient method for self-administering a medication. In an auto-injector, a syringe containing drug is accelerated by a pre-compressed spring which drives the needle into the skin and keeps the device pressed into the skin during the drug injection process. In contrast to manual injection, speeds during auto-injection can be up to 1-10m/s. Additionally, while there have been various efforts characterizing the fracture of skin and subcutaneous tissue at constant speeds [2], auto-injectors are characterized by complex dynamics which have only recently been studied in detail [3].

Here we present a computational model of auto-injection biomechanics. We capture fracture initiation, propagation, and frictional contact between fracture surfaces and needle with a cohesive zone model. A 3D model and an equivalent pair of 2D plane-strain models are presented. Skin and subcutaneous tissues are modelled as hyper-viscoelastic. To calibrate the model, data from experiments on constant needle insertion from the literature are reproduced using a combinatorial optimizer. Inferred elastic and fracture parameters from the optimization are further compared to values reported in the literature, independently of the needle insertion data. With a validated model, we fully couple the dynamic fracture model to a validated nonlinear model of an auto-injector [3]. The coupling is done through a user material subroutine in the finite element package Abaqus that calls the auto-injector model and passes the reaction force at the needle as input; it then retrieves the kinematics of the needle and enforces them in the finite element simulation.

The computational model is used to conduct a comprehensive parametric study in which both material properties and auto-injector parameters are varied. A crucial finding from this parametric study is that pre-compression by a base-plate imparts strain energy to the system, some of which is used in crack formation, reducing the force for injection. This observation in the model aligns with previous experimental work at constant needle speeds [2]. Finally, a comprehensive sensitivity analysis is carried out after replacing the expensive finite element model with an efficient yet accurate Gaussian process surrogate. This analysis is the basis for future design iterations that can robustly produce desired injection dynamics under uncertainty.

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Growth and Remodeling in Living Soft Tissues: A Statistics-based Approach

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Key Words: *Homogeneized Constrained Mixture, Statistical Modeling, Mechanobiology, Statistical Fiber Distribution*

Soft biological tissues are characterized by different cell types and extracellular matrix constituents. Structural proteins, such as collagen and elastin, are the most important ones among the extracellular components from a mechanical point of view. Collagen fibers exhibits a wide orientation distribution with the function of micromechanical reinforcement for the tissue. A striking characteristic of living soft tissues is their tendency to maintain a preferred non-stress-free mechanical state, namely mechanical homeostasis [1]. Growth and remodeling, which refer to change in mass and internal structure in living soft tissues, are crucial mechanobiological processes in developing healthy tissue and in several pathological conditions. Growth and remodeling, driven by biomechanical stimuli deviating the system from its homeostatic state, are essential to restoring mechanical homeostasis. Therefore, developing models that account for growth and remodeling is crucial to increase the insight into connections between biology and mechanics and understand the evolution of diseases.
The present work aims to develop a statistics-based approach to describe growth and remodeling in soft tissues with wide orientation distribution of fibers. Starting from the homogenized constrained mixture theory [2-3] and using the concept of mechanical homeostasis [1], we propose a probabilistic description of the fiber-mass evolution law. This description accounts for a statistical distribution of collagen fibers [4], assuming that new fibers are deposited according to a specific statistical law. We demonstrate that our framework can reproduce growth and remodeling behavior as observed in soft tissues with a statistical distribution of fiber orientations under uniaxial and biaxial loading [5].

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Mixed-dimensional Modeling of Stented Arteries using Geometrically Exact Beam Theory

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Key Words: *stented artery, geometrically exact beam theory, mixed-dimensional modeling*

Cardiovascular diseases represent one of the leading causes of death worldwide. This motivates the desire for minimally invasive procedures, reducing the risk of operative complications during arterial and coronary repairs, and accounts for the success of treatment procedures such as balloon angioplasty for stenotic arteries. Nevertheless, the occurrence of post-operative complications such as leakage, migration, restenosis, etc. frequently necessitates follow-up surgeries. The reasons for these complications are not fully understood yet. This motivates computational simulations as a tool to enhance the understanding of the underlying causes.

Computational simulation of such biomedical problems are rather complex and necessitate large system sizes to adequately capture important phenomena. Motivated by the research of Tambača et al., who utilized the benefits of 1-dimensional beam theory to efficiently simulate the behavior of coronary stents and observed a good agreement with full-dimensional models at a fraction of the system size [1], we follow the concept of modeling stents using geometrically exact beam theory. It becomes clear that not only the behavior of the stent but especially global effects of its interaction with the arterial wall and the flow around it is of interest.

This talk will demonstrate the use of highly efficient 1-dimensional stent models based on geometrically exact beam theory with a special focus on the stent's interaction with 3-dimensional continuum equations via mixed-dimensional modeling approaches as proposed in [2, 3].

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Modeling cardiac mechanics using a cell-based framework

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Key Words: *microscale cardiac mechanics, intracellular and extracellular mechanics, cardiomyocyte contraction, cell-based geometries*

Cardiac tissue primarily consists of interconnected cardiac cells which contract in a synchronized manner as the heart beats. Most computational models of cardiac tissue, however, homogenize out the individual cells and their surroundings. This approach has been immensely useful for describing cardiac mechanics on an overall level, but gives very limited understanding of the interaction between individual cells and their intermediate surroundings. Several models have been developed for single cells, see e.g. [1, 2]. In this work, we extend the mechanical part of these frameworks to a domain representing multiple cells, allowing us to investigate cell-matrix and cell-cell interactions. We present a mechanical model in which each cell and the extracellular matrix have an explicit geometrical representation, similar to the electrophysiological model presented in [3]. The strain energy functions are defined separately for each of the intracellular and extracellular subdomains, while we assume continuity of displacement and stresses along the membrane. Active tension is only assigned to the intracellular subdomain. For each state, we find an equilibrium solution using the finite element method. We explore passive and active mechanics for a single cell surrounded by an extracellular matrix and for small collections of cells combined into tissue blocks. The explicit geometric representation gives rise to highly varying strain and stress patterns. We show that the extracellular matrix stiffness highly influences the cardiomyocyte stresses during contraction. Through large-scale simulations enabled by high-performance computing, we also demonstrate that our model can be scaled to small collections of cells, resembling small cardiac tissue samples.

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Simulation of Biological Networks: Phase-field Modeling of Slime Molds

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Key Words: *optimization, finite elements, growth, fungi, infection, soft matter*

Slime molds develop macroscopic pulsating networks able to modify their structure in response to the environment. Despite their relative simplicity and the lack of a neural system, these organisms can move, solve mazes, sense nutritious or toxic agents at a distance, and even memorize periodic events. Recent studies have revealed that slime mold's pulsating unit — at the small scale — relies more heavily than previously thought on the feedback between the mechanical properties of the membrane, cytoplasm and chemical kinetics. However, the capacity to understand and replicate the emergent behavior at the level of the whole organism remains a challenge. We establish here a theoretical and computational framework to explain, quantify and reproduce how this feedback between macroscopic features and local tuning of mechanical properties determines an emergent coordinated response of the network morphology. These networks have the ability to grow, survive, or die in the presence of different concentrations of nutrients, and to redistribute them thus optimizing its proliferation. We propose a phase-field scalar variable to represent the network matrix evolution, and a diffusive-advective process for the nutrient distribution. This framework enables high fidelity simulations of slime molds in the three-dimensional space, which are challenging due to the coupled physics involved, high-order partial differential equations, and the existence of a highly complex evolving geometry. We support our simulations with experiments on a particular slime mold (*Physarum polycephalum*). The emergent properties of these organisms are similar in nature to tissues with transport networks, and can play a central role in wound healing, metastasis formation, or embryology. This investigation is a road to the microstructural design of active soft matter, object of interest in many fields of engineering and science.

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Steklov-Poincaré analysis of the basic three-domain stent problem

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Key Words: *Stents, Computational Fluid Dynamics, Multi-domain Simulations, Interface Mechanics, Domain Decomposition*

The Steklov-Poincaré problem was previously considered in the artery lumen and wall setting with a single interface. Here the analysis is expanded to incorporate solute behavior in the presence of a fixed-volume, solid, simple stent. In this geometry, a third domain is added to the two-domain structure of wall and artery. Through this intersecting domain volume setting there are three interfaces: lumen-wall, stent-lumen, and wall-stent.
Steady-state incompressible Navier-Stokes equations are used to explain the behavior of blood through the lumen, while advection-diffusion dynamics are considered for the solute mechanics across the lumen, wall, and stent. Having a fixed blood velocity value, Steklov-Poincaré decomposition of the advection-diffusion equations is applied locally to each of the interfaces. To unify these instances on a global scale, their overall intersection is explored in a smaller manifold, reducing the problem to one previously solved by Quarteroni, Veneziani, and Zunino. [1]
Through finite element analysis (FEM), the solution is discretized and found to be convergent. Finally, computational simulations of one, three, and five stent rings of different thickness, placed between straight and curved volumes of inner and outer cylindrical meshes, were performed using NGSolve, confirming the convergence of the solution and its relation to the coarseness of the mesh.

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A Multi-resolution MPS-FEM Coupling Method and Its Application to flapping flight Simulation

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Key Words: *Multi-resolution, Moving Particle Simulation Method, Finite Element Method, Fluid Structure Interaction*

In this work, a MPS-FEM coupling method is developed for the simulation of fluid-structure interaction problem, where the multi-resolution moving particle simulation (MPS) method is developed for the fluid flows and the finite element method (FEM) is employed to account for structural deformation. By using the multi-resolution MPS method, the fluid area is divided into sub-domains with different particle spacing, and an average effective radius is applied to assure the accuracy and stability. Besides, a modification is made for the kernel function to guarantee the interaction force calculation between interface particles. Then the developed multi-resolution MPS method is coupled with the FEM for fluid structure interaction simulation, where the interface force is calculated by using a volume function. By using the volume function, interaction between structures and fluid particles with different particle spacing can be solved easily, and there is no matching requirement between particle spacing and finite element size. Numerical examples are simulated to verify the effectiveness of the multi-resolution MPS method and the coupling scheme. Finally, the developed MPS-FEM coupling method will be used for the simulation of flapping flight.

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Advances in Computational Biomechanics of Insect-inspired Flapping Flights

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Key Words: *Insect-inspired flight system, flapping aerodynamics, flight stability and control, passive and active mechanism*

Flying insects power and control their flight by flapping their wings. By controlling their aerodynamic forces and torques, they can precise and agile aerial manoeuvres. From an engineer's perspective, their closed-loop, the flight control system depends on an overarching external mechanical 'frame' consisting of wings and thoracic shell, which is actuated by an internal system consisting of flight muscles and a complex nervous system [1]. Insect flights are diverse but robust relying on the integration of different flexible structures including wings, exoskeletal elements, wing-hinges, musculoskeletal elements, and sensors. In this talk I will highlight the recent advances in computational modelling of biomechanics in insect-inspired flapping flight systems with a focus on how they can offer a powerful and feasible tool to unravel a passive and active mechanism (PAM) strategy, i.e., how these flexible structures work interactively and complementarily to achieve a systematically efficient and robust flapping-wing dynamics and aerodynamics as well as flight control in various natural environments.

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Aerodynamics and Energetics in Hawkmoth Forward Flight

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Key Words: *Computational fluid dynamics, Unsteady aerodynamics, Energetics, Forward flight*

While hovering flight has been the main subject associated with flapping-wing aerodynamics, considering staying a particular point in space is very rare for most flying insects, unsteady aerodynamics and energetics associated with forward flight remain poorly understood yet. Here we address a computational fluid dynamic (CFD)-based study of flapping aerodynamics and energetics in hawkmoth forward flight over a broad range of flight velocity. We build up a wing-body morphological model of hawkmoth *Manduca Sexta* and mimic the realistic wing-body kinematics based on experimental data which enables trimmed forward flights in various forward flight velocities based on a genetic algorithm embedded with a CFD-driven aerodynamic model. Flapping forward flights are simulated with a high-fidelity CFD solver, capable of achieving precise prediction of complex vortical dynamics, both cycle-averaged and transient aerodynamic force, torque and power with a variety of flying motions and wing-body kinematics. Through the visualization of near- and far-field vortical structures, we examine the leading-edge vortex (LEV)-based mechanisms and wake topologies as well as their correlations with aerodynamic force production in various flight speeds. While the intense LEVs owing to flapping wings are responsible for creating most of the aerodynamic force, the body-based vortex induced by wing-body interaction is verified capable of augmenting the vertical force production up to 10% of the insect weight at fast velocities. The aerodynamics and energetics are further investigated in a broad parameter space in terms of aspect ratio, wing-to-body mass ratio and reduced frequency. The time-averaged body-mass-specific mechanical power exhibits a *J*-curve with increasing flight velocity, with a low level of power-consumption at most velocities but relatively high costs in hovering and the top velocity. The realistic wing-to-body mass ratio points to an obvious inflection in the power curve and high-*AR* wings can enhance the LEV production with the spanwise wing morphology matching its formation. Our results thus provide an overall understanding of the aerodynamics and energetics in various forward flights of hawkmoth, which may provide a potential design guideline for biomimetic flapping micro aerial vehicles.

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An immersed boundary regularized lattice Boltzmann method for acoustic simulations of bird-inspired FSI problems

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Key Words: Fluid-structure interaction, Flapping wings, Acoustic simulations

Fluid-structure-acoustic interaction problems are becoming more popular with the recent development of computational technologies. This numerical study focuses on developing efficient fluid-structure acoustic interaction solvers to examine birds flights. In particular, we will investigate the noise in flipping wings and experiment with some noise mitigation techniques that birds use. The work present in this paper is mainly about the development and validation of numerical methodologies. Capturing sound waves in a numerical simulation is challenging, as the length scale of sound waves is significantly smaller than that of aerodynamic fluctuations of macro variables. Thus, selecting an appropriate methodology is critical in aeroacoustic simulations. To improve the efficiency of the solving process, the lattice Boltzmann method (LBM), which describes the evolution of mesoscale velocity distribution functions, based on free-streaming and collision is used. LBM is intrinsically suitable for acoustic simulations, due to the simple nature of the solution process, large spatial resolutions and efficiency with parallel simulations. There are many different versions of LBM with distinct collision operations. The recursive and regularized (RR) BGK collision operator, which was developed based on higher-order Hermit polynomials was used to improve the numerical stability. For computations, a truncated domain is generally used. The perfectly matched boundary condition was employed at the outer domain, avoiding the nonphysical sound wave reflections. To model the fluid-solid interface of fluid-structure interaction problems, the widely used immersed boundary method was used. The von Neumann analysis was conducted investigating the stability of the regularised LBM. It was found that the accuracy and stability of the regularised LBM were improved, when the collision operator was computed from the Hermite polynomials up to 4^{th} order instead of the 2^{nd} order. In addition, two benchmark cases: the propagation of an acoustic monopole and point source and the sound generated by a stationary cylinder in a uniform flow were conducted, as validation studies. Predictions given by the IB-regularised LBM showed a good agreement with numerical simulations and analytical solutions reported in previous publications, demonstrating the capability of the IB-regularised LBM presented in this study for acoustic problems. Using the methods presented here, we will investigate the duty of separated wing-tips in noise mitigation of bird's flights in future.

Computational analysis of fluid-structure interaction in case of dragonfly flying in the vortex street

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Key Words: *Dragonfly, Fluid-structure interaction, Wing kinematics, Cylinder*

The fluid-structure interaction (FSI) in case of a live-sized dragonfly staying in the vortex street is investigated by numerical simulations. The vortex street is generated by a circular cylinder. A dragonfly model is placed on the downstream centerline of the bluff cylinder at various distances away from the center of the cylinder with considering effects of wing phase difference and wing pitching. The overset grid technology is adopted to simulate the dragonfly flapping motion. The Navier-Stokes equation in the arbitrary Lagrangian-Eulerian form is solved by coupling with the kinematics equation. Cases including stationary position with and without wing deformation are investigated. These results numerically found that, under proper conditions, the vortices can help raise the thrust force or vertical force without expending any energy of its own. This observation is also significant in the development of low-drag energy harvesting devices, and in the energetics of dragonfly clinging on long and thin pond vegetation.

Effect of Inclination Angle of Origami Winged Seeds on the Terminal Velocity and Rotation Period

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Key Words: *biomimetic, winged seed, biological fluid mechanics, terminal velocity, auto-rotation, origami technology, numerical simulation*

Bioinspired designs that imitate animals and plants' movements, behaviors, characteristics, appearance, or structure have attracted much attention due to their unique properties and potential applications to micro aerial vehicles. Examples include birds or insects, which can generate thrust and lift through flapping-wing systems [1]; wind-dispersed seeds and fruits with lightweight and flight organs such as wings that can extend the flight time and range [2]. In addition, when the Reynolds number is low, this type of flight mechanism can improve the shortcomings of current fixed-wing aircraft and may be used in topographic surveys, disaster relief operations, and military activities.

The flight mechanism of winged seeds only requires simple geometrical changes, unlike insects or birds, requiring neuromuscular control for driving [3] to reduce its descent speed. In this paper, inspired by the Dipterocarpaceae winged seeds, we use our newly-invented three-winged origami paper seeds as a model system to study the falling speed and rotation period of such bioinspired devices. We use origami winged seeds because their wing shape and angle can be readily changed to understand how they affect the flight. We changed the three-winged model's wing inclination angle, measured with respect to the horizontal plane, between 30-50 degrees. We found that when the inclination angle is smaller, the paper seeds tend to rotate at high speed and have a longer falling time in the free-fall experiment. This result is consistent with our numerical simulation. In addition, we found that the angle of the paper seeds oscillated periodically during the falling process from the simulation result. We also designed and assembled a vertical wind tunnel so that the three-winged model can fly in a specific range within the tunnel, facilitating the observation of the relationship between wing vibration, rotation period, and terminal velocity during flight.

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Estimating Lift in Flapping Flight from Wake by Using a Vorticity-Centroid Based Lift Formula

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Key Words: *Lift, Wake, Vorticity Centroid, Flapping Flight, Unsteady Aerodynamics*

The Kutta-Joukowski (KJ) theorem is usually used to estimate the lift from the wake in experimental measurements of free-flight animals. However, the KJ theorem may lead to puzzling results when it is applied to estimating the lift from the unsteady wakes [1]. We investigate this problem by using three prevalent flapping rectangular wing models [2], where the unsteady wakes are obtained by numerically solving the Navier-Stokes equations at low Reynolds numbers. The evolution of the wake and the unsteady lift generated by the flapping wing models are analysed in details. The limitations in applying the KJ theorem to flapping wings are quantitatively examined by using a simplified lift model for unsteady viscous flows [3]. It is found that neither the unsteady nor the time-averaged lift coefficient is correctly predicted when the parameters for the KJ theorem are selected according to the widely accepted ways in the literature.

We propose a vorticity-centroid wake width model based on the vortex impulse theory to improve the prediction to the lift. The proposed model computes the effective span width based on the vorticity centroid width of the wake, in which the evolutionary effects of the complex vortex structures in the wake is taken into account. When the vorticity-centroid wake width is used, the KJ theorem gives a good prediction to the time-averaged lift. Furthermore, we investigate the phase difference of unsteady lift caused by the quasi-steady assumption of the application of the KJ theorem to the flapping flight and quantitatively link the phase difference to the local fluid acceleration. We show the phase difference can be corrected by using an added mass lift model. The proposed model can be used to estimate the lift from the velocity and vorticity on a Trefftz plane in the wake. This work is helpful to clarify the error in estimating the lift of flapping flight.

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Fluid-Structure Interaction Analysis of Flapping Wing in the Martian Environment

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Key Words: Flapping wing, Fluid–structure interaction, Two-way coupling, One-way coupling, Mars

In Mars exploration, rovers often suffered from rugged areas such as cliffs and dunes, which are operationally hazardous and could be very challenging to investigate. The success of the first small helicopter, Ingenuity, by NASA has a significant impact for its demonstration that the device with rotary wings could fly in a low-Reynolds-number regime on Mars [1]. However, we consider a flapping-wing micro air vehicle (FWMAV) promising on Mars because the flapping flight is efficient in the low-Reynolds-number regime, at least on the Earth, as birds and insects take advantage of various unsteady mechanisms to achieve flight [2]. The biggest challenge for its development is an appropriate understanding of a flapping flight with flexible wings, which is significantly complicated because flexible flapping wings can undergo large-scale deformations due to the effects of wing inertia and the aerodynamic forces exerted by the surrounding atmosphere. Fluid–structure interaction (FSI) analysis is a powerful tool for accurate investigations, but it usually has a very high computational cost, making it challenging to perform necessary parametric studies for practical designing. An efficient FSI analysis method is required. On Mars, whose atmospheric density is around 1% that of Earth, aerodynamic forces have a relatively small influence on wing deformation and may even be negligible in some cases. We thus investigate the relative contributions of the inertial force of a flapping wing and the aerodynamic forces exerted by the surrounding Martian atmosphere using a two-way coupled FSI simulation [3], and identify the conditions under which the aerodynamic forces are negligible. Then, we develop a computationally efficient one-way coupled FSI analysis system based on the interface-capturing method to design a flexible flapping wing for Mars exploration [4]. Under the obtained conditions, we perform parametric studies on flexible flapping wings in the Martian environment with multiple aerodynamic parameters, various kinematic parameters, and material properties of the wing. We conclude that an FWMAV with a payload of around 5 g can fly for more than 1 minute for the maximum density of the Martian atmosphere.

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Fluid-Structure Interaction Design of Insect-Inspired Flapping Wings with 2.5-Dimensional Structure

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Key Words: *Insect Flapping Flight*, *Fluid-Structure Interaction (FSI) Design*, *Insect-Inspiration*, *2.5-Dimensional Structure*, *Computational Biomimetics*, *Passive Mechanism*, *Flapping Motion*, *Feathering Motion*, *Design Window (DW)*, *Micromachining*, *Nano Air Vehicle (NAV)*

A flight device for insect-inspired nano air vehicles (NAVs) can use the fluid-structure interaction (FSI) to create the characteristic motions of flexible flapping wings. This design concept or the FSI design will be essential for further miniaturization of NAVs, since it will reduce the mechanical and electrical complexities of the flight device.

In this study, an insect-inspired flapping wing with a 2.5-dimensional (2.5-D) structure is proposed using a computational approach for the FSI design [1], which consists of the direct numerical modelling of the strongly coupled FSI, the dynamic similarity framework, and the design window (DW) search. The proposed wing uses the passive mechanisms of both the flapping and the feathering mimicking actual insects. This wing can be fabricated using micromachining techniques based on the photolithography because of the 2.5-D structure.

The proposed wing consists of the flexible wing membrane, the leading-edge beam, and the plate spring at the base connected to a micro actuator. The membrane and spring lead to the FSI-cause of the feathering motion [2] and the resonance in the flapping motion, respectively. These motions are strongly coupled with each other. Hence, the direct numerical modelling of the strongly coupled FSI is essential in the performance evaluation of each design solution.

The flapping frequency and the lift force are taken as the design parameter and the objective function, respectively. An existing area of satisfactory design solutions or the DW [3] is searched such that each design solution in the DW can generate a sufficient lift force. In our future work, the manufacturable solutions will be selected from the DW, and they will be fabricated using the micromachining technique.

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Modeling Freely Flying Monarch Butterflies Using a Strongly Coupled High Fidelity Numerical Framework

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Key Words: *Butterfly, Unsteady Aerodynamics, Flight Dynamics, Fluid Structure Interaction*

Insects are impressive creatures due in part to their small size and agile flight maneuvers [1]. Additionally, butterflies can be highly efficient fliers, as evidenced by monarchs having the longest migration amongst insects [2]. To begin uncovering the complex mechanisms enabling monarchs to migrate roughly 80 million times their average body length, high-fidelity modeling tools must be developed. These tools must consider the distinguishing features of monarchs – their low flapping frequency, high Reynolds number (amongst insects), large wings relative to their body, low wing loading, flexibility of their wings, and the highly coupled interplay between the instantaneous wing aerodynamics and dynamic body response.

Many high-fidelity models have been used for the study of butterfly flight to date [3–5]. However, most have neglected the passive wing pitching arising from butterfly's flexible wings. Here, we propose a framework that tightly couples the effects of all three physics solvers using a dynamic relaxation scheme. As such, the highly nonlinear interplay between fluid, body, and passive wing dynamics is efficiently accounted for in each time step. We apply the model to the free flight of monarch butterflies, resulting in stable motion for many periods without any controller. Analysis of the vortex dynamics resulting from the unsteady aerodynamics coupled to the large rotations and undulations of the body will be presented.

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Relative Importance of Aerodynamic and Inertial Forces in Passive Cambering of Insect's Flapping Wings

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Key Words: *Insect Flapping Flight, Fluid-Structure Interaction, Pixel Wing Model, Passive Mechanism, Inertial Effect, Aerodynamic Effect, Cambering*

Characteristic deformations are observed in many species of insects. Especially, cambering in the flapping wings plays an important role in increasing their aerodynamic efficiency [1]. Mimicking the cambering in insect-like flapping wing nano air vehicles (FWNAVs) will increase their flight performance. It seems that the cambering is caused by the aerodynamic and wing's inertial forces (passive cambering) because of the lack of interior muscles in insect's wings. It is important to determine the relative importance of their forces in the passive cambering, which will provide an insight for the further development of insect-like FWNAVs.

Hence, in this study, the relative importance of the aerodynamic and wing's inertial forces in the passive cambering is determined using the fluid-structure interaction (FSI) analysis framework for insect's flapping wings. This framework consists of (1) a pixel wing model, which consists of a structured mesh using shell finite elements [2], and can simulate the passive cambering as well as the passive feathering, (2) a projection method [3, 4], which splits the simultaneous equation system for the FSI into two equilibrium equations and a pressure Poisson equation, and (3) the FSI nondimensional parameters [5], which can measure the dynamic similarity between the model flight and the actual insect flight.

It is shown from a numerical example using the flight data of small insects that the aerodynamic force is the basis of the passive cambering, and the wing's inertial force enhances it. In our future work, this understanding will be used in the design of insect-like FWNAVs.

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S-Version of Finite Element Method Using B-Spline Basis Function for FSI Analysis

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Key Words: *s-version of FEM, B-spline, fluid–structure interaction, flapping flight*

A considerable number of recent studies have been conducted on a numerical simulations for flapping-wing flight of a bird and an insect as a fluid–structure interaction (FSI) phenomenon. Numerical methods to deal with moving boundaries in FSI analysis can be categorized into tracking and capturing methods. However, the tracking method may generate distorted mesh for fluid domain, which makes the calculation unstable, because the flapping motion is associated with a large deformation, movement, and contact of boundaries. On the other hand, the capturing method can not maintain high-resolution boundary layer meshes for the moving boundary layers, resulting in low accuracy.
To overcome these challenges, we have extended s-version of FEM (SFEM) [1] to FSI analysis. SFEM has been studied mainly in the field of structural mechanics. In addition, we propose a new method to achieve both robustness of fluid meshes for moving boundaries and high resolution in a local domain. In this framework, we apply structured meshes based on interface capturing method to the entire domain. Higher resolution arbitrary Lagrangian–Eulerian (ALE) meshes based on interface tracking method are superimposed on the boundary layers and the surrounding area which require high spatial resolution. In addition to conventional Gauss quadrature, SFEM requires Gauss quadrature for partly superimposed finite elements with different basis functions. In SFEM, it is well known that using Lagrange polynomials as the basis functions leads to discontinuous integrand which reduces the accuracy. To solve this problem, many studies have been conducted to improve the integral accuracy by decomposing integral domains [2], but all of them are computationally expensive. In this study, we use 2nd-order B-spline function as a basis function of the structured mesh in order to make the integrand continuous and improve the integral accuracy while reducing computational cost. Numerical benchmark tests using manufactured solutions are presented to validate the numerical accuracy. Finally, the proposed method is applied to the coupled problem of flapping-wing flight.

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The Aerodynamics in Multiple Flight Modes of a Dragonfly

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Key Words: *Dragonfly, Flapping Wing, Tandem Wing, Computational Fluid Dynamics*

The effects of wing kinematics on both normal forward flight and escape flight of a dragonfly [1] are numerically investigated. A Navier-Stokes-based numerical model has been adopted and results substantiated by experimental data [2]. To shed light on the interplay between kinematics and aerodynamics, a parametric study of the kinematics has been conducted. It is found that in escape flight the dragonfly can generate additional lift while redistributing some of the thrust as well however to the expense of overall efficiency that drops by 13%. Compared to the normal forward flight, the escape mode produces larger force peaks along with higher wing loading and corresponding to more pronounced wing deformation. In escape flight wing-wing vortex interactions and downwash effects increase lift as result of mostly the changes in flapping positional angle. Regarding the phasing of the wings, in comparison with the force change caused by angle of attack variation, the influence of the phasing between fore- and hind-wing in escape flight is secondary. On the other hand, the change of angle of attack played a major role in facilitating the aerodynamic performance of normal forward flight by affecting the formation and orientation of the wing bound vortexes and directing momentum. With appropriate combination of phase and angle of attack of fore- and hind-wings, the relative magnitudes between the thrust and the lift vary. The results can help develop flight control strategies for micro scale air vehicle design.

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Abdominal and Pelvic Floor Muscles in Continent and Incontinent Women - a Biomechanical Perspective

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Key Words: *Abdominal Pelvic Cavity Muscles, Stress Urinary Incontinence, Muscle Strength*

Stress urinary incontinence (SUI), i.e., "the complaint of involuntary loss of urine on effort or physical exertion or sneezing or coughing" is prevalent in adult women. Pelvic floor muscle (PFM) strength components have been positively associated with continence (1). Stronger abdominal muscles contraction is associated with higher Intra-abdominal pressure (2). From a biomechanical perspective, woman with stronger abdominal muscles would need stronger PFM to maintain continence.

PFM strength (cmH_2O) and PFM endurance (s) were assessed by manometry. Peak torque of trunk flexor muscles (Nm), Maximal Expiratory Pressure and Maximal Inspiratory Pressure (cmH_2O) were used as a surrogate measure of superficial abdominals, deep abdominals, and the respiratory diaphragm strength, respectively.

The sample comprised 48 healthy women aged 19 to 49 years with normal Body mass index. Thirty-four were continent and 14 had SUI symptoms. The majority were nulliparous (n=42; 87.5%) and reported regular physical exercise/sport practice (n=35; 72.9%). No differences were found between continent and incontinent women in the reported variables ($p>0.05$). Regarding PFM function variables, there was no statistically significant differences in maximal strength between continent and incontinent: 62.7 cmH_2O (95% CI: 53.8 - 71.6) versus 62.6 cmH_2O (95% CI: 45.3 -80.0) p=0.725, strength: 51.9 cmH_2O (95% CI: 44.7 - 59.0) versus 55.0 cmH_2O (95% CI: 40.5 -69.5) p=0.964, and endurance 52.9 s (95% CI: 36.0 - 69.8) versus 57.2 s (95% CI: 23.7 - 90.6) p=0.812, respectively. Differences were found in abdominal cavity muscles strength between continent and incontinent: superficial abdominals 105.9 Nm (95% CI: 96.4 - 115.4) versus 128.5 Nm (95% CI: 115.7 - 141.2) p=0.005, deep abdominals 62.9 cmH_2O (95% CI: 55.6 - 70.2) versus 76.2 cmH_2O (95% CI: 65.0 - 86.4) p=0.028, and Diaphragm 61.4 cmH_2O (95% CI: 53.8 -69.0) versus 73.4 cmH_2O (95% CI: 64.1 - 82.7) p=0.048.

In this sample, no differences were found in PFM strength components between groups. Women with SUI had stronger abdominal cavity muscles strength than continents.
Should PFM strength components be considered in relation to abdominal muscles strength when evaluating women with SUI?

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Biomechanical study of abnormal uterine activity using an electro-chemo-mechanical constitutive model

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Key Words: *Vaginal Delivery, Uncoordinated Uterine Activity, Excessively Short Resting Stage, Tachysystole, Numerical Simulation, Finite Element Method*

During a normal vaginal delivery, the muscle cells propagate electrical signals throughout the uterine wall, which will result in a synchronized set of uterine contractions and resting stages [1]. An uncoordinate uterine activity may change the uterine contractions pattern and impact fetal and maternal health [2]. There are many uterine activity abnormalities identified by the specialists, such as precipitate labor, excessive frequency of contractions (tachysystole), excessive contraction duration, excessively short resting intervals, among others.

The main goal of this work is to investigate the maximum principal stress distribution and the collagen fibers stretch in the uterine tissue during a vaginal delivery with (i) a normal contraction pattern, (ii) excessively short resting intervals and (iii) excessively uterine high frequency (tachysystole).

A biomechanical model comprising a fetus and a uterus was developed and an electro-chemo-mechanical constitutive model that triggers uterine contractions was implemented and validated with literature findings. The normal contraction pattern was defined with a contraction time of 80s and a resting time of 60s, while for the excessively short resting interval the contraction time was maintained, and the resting stage was shortened to 20s. Finally, the tachysystole was characterized by a contraction time of 55s and a resting stage of 35s.

Generally, the excessively short resting intervals exhibit higher average maximum principal stresses during the contraction and resting stages, lower average fibers stretch values in the longitudinal direction, and higher stretch in the circumferential direction. This indicates that more intense uterine contractions will be created, which my interfere with the fetal oxygenation, since higher contractions tend to compress the uterine vessels. On the other side, the tachysystole exhibit generally lower stress values during the uterine contraction and higher stress values during the resting stages, higher stretch in the longitudinal direction and lower stretch in the circumferential direction. Once more, oxygenation deficiency may be detected, since the uterine muscle does not have time enough to rest, leading to higher stresses at the end of each resting interval.

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Computational modeling of a fetal malposition during a maternal flexible-sacrum birthing position

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Key Words: *Childbirth biomechanics, Finite element model, Pelvic floor dysfunctions, Fetal positions*

Childbirth can be a mechanically traumatic event. The impact of the fetal position on women and neonates is considerable, with high rates of birth trauma associated with occipito-posterior (OP) positions [1]. The main goal of this study is to analyze the influence of a persistent OP malposition on the maternal pelvis and pelvic floor, with the mother assuming a flexible-sacrum birthing position.

A finite element model was used to simulate vaginal delivery in the vertex presentation. The mother's model includes the pelvic floor muscles (PFM), hip bones, sacrum, coccyx, and main pelvic ligaments [2, 3]. The movement of the coccyx around the sacrococcygeal joint is allowed, to mimic maternal positions in which the weight of the body is off the sacrum. The fetus is composed of the skin, skull, brain, sutures, and fontanelles [4]. Two simulations were performed in Abaqus® software to mimic the fetus in occipito-anterior (OA) and OP positions. To evaluate the effect of distinct fetal positions, the stretch, maximum principal stresses, and coccyx rotation were analyzed.

The maximum principal stresses were measured at different paths of the PFM and were higher for the OP position. The major difference was an increase of 55.20% in the OP position compared to the OA. The coccyx rotation in the OA and OP positions was, respectively, 0.98º and 2.17º. The fetus has more difficulty progressing in the OP position since the maximum muscles' stretch is achieved at a later stage.

Childbirth is a complex biomechanical process that can put both mother and fetus at risk of injuries. The maximum principal stresses obtained indicate that the muscles are subjected to higher stresses in the OP position at the instant of maximum stretch. These results demonstrate that the OP is more demanding for the PFM, corroborated by previous numerical and clinical studies [5]. Furthermore, in the OP position the coccyx needs to rotate twice as much as the OA position for the fetus to progress. In clinical terms, the OP position appears to be more demanding for the mother's pelvis. To conclude, the current work demonstrates that the OP position can be harmful to the pelvic floor muscles during a flexible-sacrum maternal position.

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Improving Childbirth Outcomes: A Biomechanical Approach

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Key Words: *Occiputanterior position, Occiputposterior position, Childbirth-related injuries, Numerical simulations*

Despite being a natural physiological event, childbirth is a very complex process that can have a negative impact on women. Childbirth-related trauma impacts millions of women and babies worldwide [1]. Pelvic floor muscle injury, both micro and macrotrauma, has an incidence of 10-36%, and anal sphincter injury of 4-6.6% [2]. Pelvic floor injuries are exacerbated by fetal malposition, such as persistent occiputposterior (OP) position, which is estimated to affect 1.8-12.9% of pregnancies [3]. Childbirth-related trauma plays an important role in the development of pelvic floor dysfunction, and diagnosis rates at the time of injury are still poor [4].

The biomechanical aspects of childbirth are still not entirely understood; as such, computer models aim to improve current knowledge by evaluating mechanical aspects during vaginal delivery, such as stress, strain, forces and contact pressures. A 3D biocomputational model previously developed to simulate vaginal deliveries was used in our studies, including the mother and the fetus [5]. The birthing process is a complex physiological phenomenon, so it is important to have a representative anatomical model to perform accurate biomechanical simulations. From our studies, we realized that the OP position induces a greater increase of the anteroposterior diameter. Furthermore, the maximum value occurs at a higher location in the birth canal compared to the normal position (occiputanterior, OA). This need for longer stretches at an earlier time of fetal descent can be a reason for prolonged second stage of labor in case of fetal malposition. The OP position is more demanding for the pelvic floor muscles than the OA position, corroborated by clinical studies [5]. On the other hand, the OP position was considered biomechanically favorable to the fetus since it suffers less head deformations. The molding index, which evaluates the variation of predefined diameters of the fetal head, shows significantly lower values for the OP position compared to the OA position.

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Uterine prolapse repair surgery: A computational analysis

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Key Words: *Finite Element Methods, Pelvic Cavity, Pelvic Organ Prolapse, Surgical Implants, Anchoring Technique*

The uterosacral (USLs) and cardinal ligaments (CLs) are the primary pelvic structures that provide apical support to the upper vagina and uterus [1]. The impairment of these connective tissues is strongly associated with pelvic organ prolapse (POP), namely the uterine prolapse, that has long been studied [2]. The prevalence of POP, which is now up to 41.1%, is likely to increase due to improvements in overall healthcare and increase life expectancy [3].The synthetic implants are used for the reconstructive surgery of POP, but severe complications associated with their use have been reported, mainly related to their mechanical properties.

In this study, we mimicked a transvaginal reconstructive surgery to repair/replace the apical ligaments (USLs) and CLs), by modeling, after their impairment and/or total rupture, respectively. The implants to reinforce/replace these ligaments were built based on literature specifications and their mechanical properties were obtained through uniaxial tensile tests. Additionally, the effect of mesh anchoring technique (simple stitch and continuous stitch) was analyzed.

The absence/presence of the synthetic implant was simulated when total rupture of the CLs and USLs occurs, causing a variation of the vaginal displacement (9% for the CLs and 27% for the USLs). The simulations also showed that there was a variation of the supero-inferior displacement of the vaginal wall between different anchoring techniques, being approximately of 10% for the simulation USLs and CLs implant.

The simulation was able to mimic the biomechanical behavior of the USLs and CLs, in response to different anchoring techniques, which can be help improving the outcomes of the prolapse surgery in the future.

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Modeling Intracellular Transport and Traffic Jam in 3D Neurons Using PDE-Constrained Optimization

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Key Words: *Neuron intracellular transport, Traffic jam, Microtubule swirls, PDE-constrained optimization, Isogeometric analysis*

The intracellular transport process plays an important role in delivering essential materials throughout branched geometries of neurons for their survival and function. Many neurodegenerative diseases have been associated with the disruption of transport. Therefore, it is essential to study how neurons control the transport process to localize materials to necessary locations. Here, we develop a novel optimization model to simulate the traffic regulation mechanism of material transport in 3D complex geometries of neurons. The transport is controlled to avoid traffic jam of materials by minimizing a pre-defined objective function. The optimization subjects to a set of partial differential equation (PDE) constraints that describe the material transport process based on a macroscopic molecular-motor-assisted transport model of intracellular particles. The proposed PDE-constrained optimization model is solved in complex tree structures by using isogeometric analysis (IGA). Different simulation parameters are used to introduce traffic jams and study how neurons handle the transport issue. Specifically, we successfully model and explain the traffic jam caused by reduced number of microtubules (MTs) and MT swirls. In summary, our model effectively simulates the material transport process in healthy neurons and also explains the formation of a traffic jam in abnormal neurons. Our results demonstrate that both geometry and MT structure play important roles in achieving an optimal transport process in neuron.

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Multi-scale Simulations of Pulmonary Airflow based on a Coupled 3D-1D-0D Model

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Key Words: Multiscale modeling, Pulmonary airflow simulation, Respiratory system, Mixture theory

In this study, a 3D-1D-0D multiscale method is developed for simulating pulmonary airflow. Airflow in the respiratory bronchioles and alveoli were calculated by a two-phase mixture model (0D) coupled with the lung deformation. The terminal bronchioles were approximated by a pipe model (1D) which is connected with the 0D lung parenchyma. Such strong coupled 0D-1D system is solved by finite element method. For the airflow inside the trachea and bronchus, a three dimensional (3D) computational fluid dynamics analysis was performed by finite volume method based on the real bronchial geometry extracted from CT images (3D). The multi-scale respiratory simulation system was realized by satisfying the mass and momentum conservation law. In addition, the continuous condition of pressure was also ensured at the terminal nodes of the 1D airways and the corresponding mesh central points of 0D mixture solid. The coupling between 3D bronchus and 1D terminal bronchioles is conducted by transferring the information of the flow rate and pressure between the 3D bronchial terminal's outlets and the connected 1D bronchioles inlets. Such data transfer is performed by a serial staggered fashion. Therefore, the overall 3D-1D-0D coupling algorithm belongs to the class of two-way weakly coupling type. The results showed the same changed lung volume with the volume of inhalation flow, which demonstrated the mass conservation condition. Moreover, to consider the effect of airway deformation on the airflow patterns, we extracted the displacements of airway wall from the elements of surrounding lung parenchyma. A dynamic mesh method was then employed to describe the temporal and spatial nodal displacements of the whole 3D airway domain. The results indicate that the airway deformation has an apparent influence on the airflow structure in the respiratory system.

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PDE-preserved learning architecture for predicting spatiotemporal dynamics based on differentiable programming

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Key Words: *Geometric deep learning, differentiable programming, Surrogate modeling*

The recent development of physics-informed deep learning (PiDL) that leverages domain knowledge and physical prior has shown promise in solving physical problems in many science and engineering fields. In most existing PiDL works (e.g., physics-informed network, or PINN), physics prior knowledge is mainly utilized to inform or constrain the training process of the network by incorporating known governing equations into the loss function in a soft manner. However, the mathematical understanding of the system has not been fully leveraged, for example, in network architecture design. In this work, we develop a novel physics-informed deep learning architecture for predicting spatiotemporal dynamics. The network construction, layer connections, and output constraints are based on the discretized structure of the governing partial differential equations (PDEs). The learned model can be used as a parametric surrogate model for the fast prediction of spatiotemporal dynamics, facilitating UQ analysis in high-dimensional complex systems. We will demonstrate the proposed method on cardiovascular biomechanics, where the geometries of the problems are complex and irregular. In particular a statistical generative model for 3-D patient-specific shapes will be constructed based on a handful of available baseline patient geometries. An unsupervised shape correspondence solution is used to enable geometric morphing and a compact geometric design space can then be constructed by the statistical generative shape model. With the fast surrogate model, we demonstrate its application in shape optimization and UQ analysis in a massively scalable manner.

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Physics-Informed Data-Driven Parameter Identification of Human Musculo-Skeletal Systems

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Key Words: *Physics-informed neural networks, parameter identification, human musculo-skeletal motion*

The motion of human musculo-skeletal (MSK) systems result from a complex interaction of the neural signals that activate the muscles leading to forces produced by the length and velocity changes from the contraction of muscle tendon units. These forces produce torques at the joints (joint kinetics), updating the joint angles and velocities (joint kinematics) resulting in the controlled movement of the human MSK system. In practise, for analysing the motion of a specific subject, the muscle activation can be estimated by using surface electromyography (EMG) signals whereas the muscle tendon force generating properties can be obtained by using parameterised hill-type models. These parameters are identified by solving an optimization problem with given motion capture data, in which the algorithms for calibration can be computationally expensive. In this work, a physics-informed data-driven framework for parameter identification of human MSK systems is proposed, where neural networks enhanced with physics-based constraints are employed. Specifically, residuals of governing differential equations are penalized in the loss function for a more robust system identification procedure satisfying the underlying physics, such as both joint kinetics and joint kinematics. The proposed framework is examined by identifying parameters in muscle models given subject specific EMG and motion data, where the identified parameters of the subject are then compared against physiological estimates. Future work to enhance the framework using continuum level muscle-tendon behaviours as well as medical imaging data is also highlighted.

Shear Induced Cell Damage: Multiscale Modelling and Experimental Validation

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Key Words: *Multiscale Modelling, Coarse Grained Molecular Dynamics, Cell Squeezing*

Shear stress in medical devices such as ventricular assist devices and microfluidic devices can be significantly higher than physiological range, leading to damage of cells. Under these high shear stresses, cells experience sublytic damage, which is temporary pore forms allowing cellular content to release or outside agent to delivery in, or in more critical cases, complete rupture and apoptosis of cell. Cell damage can cause serious problems like anemia, arrhythmias, stroke for hemolysis of red blood cells, or immune response for white blood cells. However, transient cell damage is also widely used for intracellular delivery of drugs and agents into cells, yet the underlying mechanics is not well understood. We developed a cellular model of cell damage through multiscale modelling and experimental characterization. This a bottom-up cellular model, in contrast with the present continuum approaches, is not device-dependent, thus can predict cell damage and agent delivery in any device. At the continuum scale, computational fluid dynamics (CFD) simulations are used to get the shear stress history of individual cells passing. Mesoscale fluid-structure interaction simulations is performed to determine the critical threshold of pore formation and geometrical characteristics of pores under various loading conditions. Coarse-grained molecular dynamics (CGMD) simulations of pore formation in a membrane patch that explicitly includes both lipid bilayer and cytoskeleton particles are used to develop the subcellular damage model. The critical strain and dynamic process of pore formation under physiologically strain/shear rates are quantified. The cell damage and intracellular delivery are found to be a function of shear stress and exposure time. Finally, the cell damage during squeezing through microfluid channels of various widths and length was studied experimentally. The simulated cell damage agrees well with experimental results.

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A Fully Coupled Thermo-Hyperelastic Constitutive Model of Myocardium: The Role of Thermoelastic Anisotropic Conduction and Cellular Death During Radiofrequency Catheter Ablation

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Key Words: Constitutive model, Myocardium anisotropy, Radiofrequency catheter ablation, Cellular death dynamics, Multiphysics couplings, Finite Element Analysis

Radiofrequency catheter ablation (RFCA) is an effective treatment for various types of cardiac arrhythmias [1]. However, constitutive models of RFCA lack a reliable three-dimensional microstructural representation of the tissue. In the present work, we propose a novel transverse isotropic thermo-hyperelastic constitutive model of the myocardium fully coupled to the thermo-electrical problem arising from the RF procedure. We account for the local anisotropy in the thermo-electrical conduction mechanisms and employ a three-state cell death model including mechanical damage. We implemented a two-way coupling between the mechanical and heat transfer model at the constitutive level through the multiplicative decomposition of the deformation gradient. A thermoelastic equation for the heat transfer model, consistent with generalized thermodynamics-based constitutive theories [2], is further advanced. We numerically solved the multiphysics problem within an idealized tissue domain, adopting a mixed finite element scheme augmented by a constant power constraint for the RFA procedure. Remarkable results include: (i) the elliptically-shaped thermal lesions; (ii) stiffening of the tissue; (iii) a residual tensional state due to damage accumulation. These results offer compelling evidence for enhanced predicting capabilities of RFCA numerical models, including microstructural features of the tissue and multiphysics coupling with the clinical procedure. We discuss future developments, including viscous dissipation and generalized remodel theories, as well as an extensive clinical validation that is foreseen to confirm the application of our approach to device design and therapeutic optimization.

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A new computational model to study mechanisms governing e-cadherin-based cell-cell adhesion junction formation and maintenance

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Key Words: *Adherens junction, computational model, cadherin, actin, cell adhesion*

Adherens junctions (AJs) are protein complexes at the cell-cell interface that withstand mechanical forces and maintain tissue structure. They also regulate intracellular signalling for cell growth, division and death. Proper adherens junction structure and function is therefore critical for tissue development. Adherens junction dysfunction causes cancer metastasis. Deciphering the molecular regulators of adherens junctions is challenging partly because of complex interactions between mechanical forces and chemical signals within the junction. Unravelling the interactions would help identify potent targets for cancer therapies and also help advance technologies like bioprinting and regenerative medicine.

AJs involve extracellular bindings between cadherin molecules and intracellular interactions between cadherins and the actin cytoskeleton. Both cadherin and actomyosin cytoskeletal dynamics are reciprocally regulated by mechanical and chemical signals, which subsequently determine the strength of cell-cell adhesions and the emergent organization and stiffness of the tissues they form. However, an understanding of the integrated system is lacking.

We present a new mechanistic computational model of intercellular junction maturation in a cell doublet to investigate the mechano-chemical crosstalk that regulates AJ formation and homeostasis. The model couples a 2D lattice-based model of cadherin dynamics with a continuum, reaction-diffusion model of the reorganizing actomyosin network through its regulation by Rho signaling at the intercellular junction. We demonstrate that local immobilization of cadherin induces cluster formation in a cis less dependent manner. We then recapitulate the process of cell-cell contact formation. Our model suggests that cortical tension applied on the contact rim can explain the ring distribution of cadherin and F-actin on the cell-cell contact of the cell-doublet. Furthermore, we propose and test the hypothesis that cadherin and F-actin interact like a positive feedback loop, which is necessary for formation of the ring structure. Different patterns of cadherin distribution were observed as an emergent property of disturbances of this positive feedback loop. We discuss these findings in light of available experimental observations on underlying mechanisms related to cadherin/F actin binding and the mechanical environment.

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Mixed methods for large-deformation poroelasticity and application to oedema formation

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Key Words: Poroelasticity, Multiphysics Problems, Biomedical Applications

In this talk we propose a novel coupled poroelasticity-diffusion model for the formation of extracellular oedema and infectious myocarditis valid in large deformations, manifested as an interaction between interstitial flow and the immune-driven dynamics between leukocytes and pathogens. The governing partial differential equations are formulated in terms of skeleton displacement, fluid pressure, Lagrangian porosity, and the concentrations of pathogens and leukocytes. A similar model with applications in morphogenesis is also discussed.

A five-field mixed-primal finite element scheme is proposed for the numerical approximation of the problem, and we provide the stability analysis for a simplified system emanating from linearisation. We also discuss the construction of an adequate, Schur complement based, nested preconditioner. Numerical tests exemplify the properties of the new model and of the mixed schemes.

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Thermo-mechanical Effect of Excitable Lipid Dynamics in Spatially Confined Cell Membranes

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Key Words: *PtdInsP3, Dictyostelium, Stochastic Simulations, Membrane Curvature, Diffusion, Plasma Membrane, Pattern Formation*

PtdInsP3 lipid signalling is essential for regulative processes in *Dictyostelium* and mammalian cells. Recently, it has been experimentally shown that waves of PtdInsP3 are solely self-regulated through the mechanical deformation of the plasma membrane even in the absence of the regulative actin network. The dynamics are defined by the underlying excitability and the shape of the membrane, leading to horizontal and vertical, as well as transient spot dynamics of PtdInsP3 domains[1]. Further, it was shown that the diffusion of t hose domains are strongly influenced by strongly curved membranes, as it is observed at the leading edge of protrusions and macropinocytic cups[2].

In order to fully understand the experimental observations, we investigate the thermo-mechanical effects of the PtdInsP3 lipid signalling *in-silico* with realistically shaped three-dimensional plasma membranes, as observed *in-vitro*[1], an experimentally based reaction-diffusion scheme [1, 3] and the stochastic τ-leap method to simulate the PtdInsP3 domain dynamics [4]. We found that the variation of membrane deformation, excitability and curvature dependent diffusion regulates the PtdInsP3 lipid signalling, and can recover fundamental system dynamics as observed in experiments.

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A SYSTEMATIC COMPARISON OF REDUCED-ORDER MODELLING AND PHYSICS INFORMED MACHINE LEARNING TECHNIQUES TO ACCELERATE ONE-DIMENSIONAL BLOOD FLOW COMPUTATIONS

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Key Words: *Deep neural network, Blood flow modeling, Reduce-order modeling*

One-dimensional blood flow modeling has proven to be a powerful tool to capture flow and pressure waveforms in complex vascular networks. Despite its computational efficiency, the existing developments are still far from achieving real-time, especially in large vascular networks, and keeping in mind the large number of time steps required to model a single cardiac cycle. Additionally, one-dimensional models typically rely on the use of 0 D lumped parameter models to capture the effect of the truncated vasculature at each of the model outlets. This turns into dozens of parameters to be estimated at the patient-specific level. Overall, this still results in computationally intensive simulation pipelines, incompatible with the stringent clinical time frame.

In the last years, a wealth of techniques have been proposed to accelerate computational physics simulations via machine learning. These techniques fall into two large groups. From one side, non-intrusive reduced-order modeling techniques, which typically use a (sufficiently) large dataset of simulations to extract, via proper orthogonal decomposition, intrinsic similarities of the solutions and project them into a lower-dimensional space. Then, machine learning (neural networks, Gaussian process regression) is used to find the nonlinear relationship between model parameters and the solution on the reduced space. On the other side, physics-informed machine learning is based on building a neural network architecture aimed to replace the computational physics model via enforcing the satisfaction of the driving physical laws. More recently, techniques that combine the two approaches have also been proposed.

Whereas these techniques are very promising, their relative advantages and disadvantages remain unclear. This work aims at comparing different machine learning-based reduced-order modeling, physics informed machine learning, and hybrid methods for accelerating one-dimensional blood flow simulations. The methods will be compared in terms of accuracy of the predicted solution, the satisfaction of the underlying physical laws, required offline training time, and computational speed-up in the on-line evaluation. To do so, a set of models based on idealized and patient-specific geometries will be used to extract relevant conclusions.

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Assessment of stroke risk in pediatric cerebrovascular disease through patient-specific modeling

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Key Words: *Computational fluid dynamics, Isogeometric analysis, Moyamoya, MRI, Wall shear rate score*

Background and Purpose. Moyamoya disease (MMD) is a progressive steno-occlusive cerebrovascular disease leading to recurrent stroke. There is a lack of reliable biomarkers to identify unilateral stroke MMD patients who are likely to progress to bilateral disease and experience subsequent contralateral stroke(s). We hypothesized that local hemodynamics are predictive of future stroke and set out to noninvasively assess this stroke risk in pediatric MMD patients.

Methods. MR and X-ray angiography imaging were utilized to reconstruct patient-specific models of the circle of Willis of 6 pediatric MMD patients who had previous strokes, along with a control subject. Blood flow simulations were performed by using a Navier-Stokes solver within an isogeometric analysis framework. Vascular regions with a wall shear rate (WSR) above the coagulation limit ($> 5000\ s^{-1}$) were identified to have a higher probability of thrombus formation, potentially leading to ischemic stroke(s). Two metrics, namely, "critical WSR coverage" and "WSR score", were derived to assess contralateral stroke risk and compared with clinical follow-up data.

Results. In two patients that suffered a contralateral stroke within two months of the primary stroke, critical WSR coverages exceeding 50% of vessel surface and WSR scores greater than 6x the control were present in multiple contralateral vessels. These metrics were not as conclusive in two additional patients with 3-to-5-year gaps between primary and contralateral strokes. However, a longitudinal study of one of these two cases, where a subsequent timepoint was analyzed, accurately predicted disease stabilization on the primary stroke side and an elevated contralateral stroke risk, thus indicating that post-stroke follow-up at regular intervals might be warranted for secondary stroke prevention.

Conclusions. WSR-based metrics could be predictive of future stroke risk after an initial stroke in MMD patients. In addition, more accurate predictions may be possible by performing patient-specific hemodynamic analysis at multiple timepoints during patient follow-up to monitor changes in the WSR-based metrics

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Data-driven reduced order models for cardiovascular simulations

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Key Words: Reduced-order models, neural networks, cardiovascular simulations

We are interested in learning reduced-order models for cardiovascular applications from high-fidelity 3D simulations. We are motivated by the fact that traditional physics based reduced-order models—e.g., 0D and 1D models—can suffer from loss of accuracy in complex geometries (featuring, for instance, many bifurcations and/or pathological conditions such as stenoses) [1]. We first consider a combined domain-decomposition and Proper Orthogonal Decomposition (POD) approach; here, the target geometry is approximated by simple geometrical building blocks equipped with a low number of basis functions for velocity and pressure. In [2], we show that this approach is accurate in approximating velocity, pressure and wall-shear stress, and leads to significant speedup (at least 10 times) with respect to the Finite Element Method (FEM). We also consider a machine learning method trained on a large dataset of high-fidelity simulations available in the Cardiovascular Biomechanics Computational Lab at Stanford University, the Vascular Model Repository (VMR). We develop a surrogate 1D solver based on graph neural networks (GNNs) by following a strategy similar to that presented in [3]. In each timestep of our method, the GNN encodes, processes and decodes the flowrate and pressure values located at the nodes on the centerline of the cardiovascular model and outputs the updated state of the system. We will present comparisons with standard 1D reduced-order and high-fidelity simulations and highlight the strengths and challenges of our approach.

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DISCOVERY OF REDUCED ORDER MODELS FOR FLOW THROUGH A CORONARY STENOSIS

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Key Words: Reduced Order Model, Computational Fluid Dynamics; Data-driven Modeling

Coronary artery disease is characterized by a narrowing or stenosis in the vessel. Fractional flow reserve (FFR), a measure of stenosis severity, is the pressure gradient across a stenosis and is measured by an invasive and technically challenging procedure. Developing a computational method to estimate FFR avoids risks associated with this procedure; however high-fidelity (3D) models are computationally expensive and impractical for real-time diagnosis. Low fidelity models based on 1D nonlinear theory are computationally inexpensive[1], but cannot fully characterize the complexities of the flow across a stenosis. In this project, we aim to develop a reduced order model (ROM) capable of accurately describing the complexities of flow across a coronary stenosis.

An ensemble of precomputed solutions can be represented on a graph, where each node is a separate boundary value problem. This allows the use of nonlocal calculus to calculate the terms for a library of candidate operators[2]. The terms we choose to include in the candidate library are based on techniques such as polynomial expansion of the quantities of interest. We also include terms based on existing models of the pressure gradient across a stenosis[3]. Terms from this library are eliminated through stepwise regression until the loss reaches a Pareto front. The new model is identified as the most parsimonious one on the Pareto front.

To validate this approach, we started with a problem with a known analytical solution, laminar flow through a pipe. We successfully recovered the known model for the pressure gradient, i.e., Poiseuille flow. The methods presented are a preliminary proof of concept for generating a reduced order model using a graph theoretic approach. These methods will be used for models of increasing geometric complexity, from a tapered pipe, to an idealized stenosis, to a more realistic stenosis with curvature.

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Effect of Non-sinus-matching Bioprosthetic Aortic Valve Design on Coronary Flow

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Key Words: Sinus-matching, Bioprosthetic valve, Fluid structure interaction, Parametric modeling

Technological advances in medical imaging and computer simulations have made it possible for us to better understand the cardiovascular system. Even though there are several morphologies of the aortic cusps in the native anatomy of a healthy heart, the leaflets always match the sinuses of Valsalva. Recent studies have shown that the mechanism of aortic leaflet closure is correlated with the formation of the vortices in the sinus of Valsalva. These vortices allow the cusps to open and close while exerting a fluid dynamic control mechanism that positions the cusps away from the aorta wall, and the slightest reversed flow in the ascending aorta will close the valve [1]. Bioprosthetic aortic valve interventions change the hemodynamic behaviors of the heart and the formation of these vortices. While there have been efforts to design asymmetric frames to better match the aortic annulus, the effect of sinus-matching leaflet design has not been investigated. In this work, we present a comprehensive framework for designing axially asymmetric/symmetric stented prosthetic aortic valves and aortic roots using parametric geometry and Fluid-Structure Interaction (FSI) analysis [2, 3]. We investigate the effects of a sinus-matching leaflet design in an axially asymmetric aortic valve configuration and compare it to the conventional axially symmetric leaflet design. We look at the orifice and coaptation areas quantitatively and the vortex formations qualitatively. This framework can be ultimately used to design optimal bioprosthetic aortic valves that match the sinus geometry for a given patient, leading to better hemodynamic performance of the left cardiac system.

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Geometric deep learning and statistical shape modeling for fast surrogate CFD simulations of patient-specific hemodynamics

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Key Words: *Patient-specific CFD, surrogate modelling, machine learning, UQ*

Optimization and uncertainty quantification (UQ) have been receiving an increasing amount of attention in computational hemodynamics. However, existing methods based on principled modeling and classic numerical techniques have faced significant challenges, particularly when it comes to complex 3D patient-specific shapes in the real world. First, it is notoriously difficult to parameterize the input space of arbitrarily complex 3-D geometries. Second, the process often involves massive forward simulations, which are extremely computationally demanding or even infeasible. We propose a novel deep learning solution to address these challenges and enable scalable geometric UQ and optimization. Specifically, a statistical generative model for 3-D patient-specific shapes will be constructed based on a handful of available baseline patient geometries. An unsupervised shape correspondence solution is used to enable geometric morphing and a compact geometric design space can then be constructed by the statistical generative shape model. In order to build a fast forward map between geometric input space to the solution space of functional information, we propose a supervised deep learning solution. With the fast surrogate model, we ran test cases to demonstrate its application in shape optimization and UQ analysis in a massively scalable manner.

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Identifying the Biomechanical Properties of a Flexible Thrombus

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Key Words: Thrombosis, Inverse Problems, Phase Field Model, Computational Fluid Dynamics

Modelling thrombosis with numerical simulations remains as a challenging task [1] consisting of multi-physics, multiscale, and complex fluid dynamics with fluid-structure interactions. In this work, we focus on the problem of identifying the mechanical properties of developed thrombi within blood vessels, using the dynamics of the interface between blood flow and thrombi.

A viscoelastic porous medium was assumed for the thrombus because of its fibrous network. The fluid-structure interaction between the thrombus and blood flow was modelled in the Eulerian reference frame using the Cahn-Hilliard and Navier–Stokes equations [2]. Two biomechanical properties of the thrombus, specifically the permeability and viscoelastic modulus, was identified with an inverse model using a twin experiment approach. Synthetic results were first generated with a prescribed permeability and viscoelastic modulus, and then second an optimiser was employed for minimising the difference between the simulated and synthetic thrombus interface. Such a method of parameter identification has previously been used elsewhere, including for describing temperature-dependent lava rheology [3].

We discuss the sensitivity of biomechanical properties to the thrombus dynamics, and the robustness of the inverse method by adding noisy data to imitate experimental uncertainties. Finally, we compare our results with recent work using physics-informed neural networks [4].

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Image-to-Analysis for Gated Volumetric Echocardiography

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Key Words: echocardiography, machine learning, image-to-analysis, image segmentation, SimVascular

Despite numerous advances in diagnosis and treatment, cardiac disease (CD) remains the leading cause of death in the United States. Prevention and early diagnosis of CD often requires monitoring of the heart itself. Monitoring is typically accomplished through echocardiographic (i.e., cardiac ultrasound) screening due to its accessibility, cost-effectiveness, real-time capabilities, and demonstrated prognostic value.

Identifying and evaluating biomarkers for CD depends on efficient segmentation and analysis of echocardiographic images. Processing these images can be time-consuming, expensive, and error-prone due to reliance on expert human technologists and radiologists. Automation of MR and CT image processing using deep learning has shown significant promise, but processing of volumetric ultrasound data has lagged behind other modalities due to its lower signal-to-noise ratios, lower image contrast, bone and gas image artifacts, and organ boundary uncertainty. For example, open-source image-to-analysis toolkits like SimVascular can automatically process cardiac MR and CT images [2], but this functionality is not supported for echocardiographic data [3].

In this talk, we will present ongoing work in our comprehensive investigation of automatic segmentation methods for 3D and 4D echocardiographic images [1]. We will show how these echo segmentations can serve as patient and mouse-specific geometry in blood-vascular and blood-heart simulations in SimVascular. Then, we will present novel regional geometric and biofluidic biomarkers of cardiomyopathy obtained from mouse and human data sets.

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Immersed Discrete Element Method With Applications In Embolus Transport

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Key Words: Fluid Structure Interaction, Discrete Element Method, Biomedical Applications

Fluid-particle interaction phenomena in complex domains are prevalent in many physiological and biomedical applications. One important application concerns the transport of emboli in a large artery, where the complexity of embolic particle dynamics and their interaction with complex pulsatile flow structure inside large arteries renders significant challenges in predicting the transport of such particles. This problem is particularly important for arterial embolisms, where knowledge of embolus transport to major blood vessels helps in diagnosis and treatment planning for stroke and other major cardiovascular diseases. Despite several existing approaches to handle two-way coupled fluid-particle interaction, simultaneous coupling for a multi-particle system in a complex physiological flow domain remains a challenge. In this work, an implementation of a coupled fluid-particle interaction algorithm for a complex multi-particle system is presented. The two-way coupled fluid-particle interaction is resolved using an immersed finite element method in which the particle domain is represented as a Lagrangian mesh moving on top of a fixed Eulerian fluid mesh [1, 2]. This allows for the fluid mesh to be generated independently from the solid structure, thereby simplifying the meshing process for multi-particle systems. The no-slip condition and interaction force at the fluid-particle interface is enforced using a mesh-to-mesh interpolation via finite element basis function transformation. Support size on which the fluid-structure interaction force is applied is commensurate with size of elements touching the particle domain and therefore optimal in an element-wise sense. Each immersed inertial particle is treated as a discrete element interacting with other particles or domain boundaries. In this presented work, particle-particle and particle-wall interactions are handled using a Hertzian elastic body collision model. Results from two canonical particle-laden flows problems are presented to validate the implementation, followed by simulations for a two-way coupled embolus transport simulation inside a physiologically realistic vessel.

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Multiphysics and multiscale models for the numerical simulation of the cardiac function

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Key Words: Heart modeling, Multiphysics and multiscale models, Numerical simulations, Computational Medicine

We present recent advancements on multiphysics and multiscale models for the numerical simulation of the whole cardiac function. In particular, we detail our contributions to cardiac electromechanics of the ventricles and then of the whole heart. Specifically, we couple state–of–the art models for the electrophysiology of the tissue, mechanical activation at the cellular level, and the passive mechanical response of the muscle, thus yielding a coupled electromechanical problem within the active stress paradigm. Our multiscale model for cardiac electromechanics accounts for miscroscopic active force generation at the cellular level by means of model order reduction based on Machine Learning algorithms. In addition, our 3D electromechanical model is coupled with a 0D, closed-loop model of the systemic and pulmonary blood circulations, other than of the other cardiac chambers. We consider the space approximation of the Partial Differential Equations therein involved by means of the Finite Element method. We numerically solve the coupled electromechanics problem by exploiting intergrid transfer operators, as well as partitioned–staggered schemes for realizing the numerical coupling. We present and discuss numerical simulations, obtained in the high performance computing framework, of cardiac electromechanics problems in the human heart, both in physiological and pathological conditions. Finally, we also present a Machine Learning method that enables real-time numerical simulations of cardiac electromechanics.

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Quantifying the Range of Mechanical Stimuli from the Severity and Duration of Aortic Coarctation that Prevents Permanent Vascular Remodeling

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Key Words: *Coarctation of the aorta, Congenital cardiovascular defects, Hypertension, Fluid-structure interaction*

Coarctation of the aorta (CoA) is one of the most common congenital cardiovascular (CV) defects. Surgical repair of the coarctation is used to enhance lifespan from CV morbidity [1], but life expectancy is still lower than normal mainly due to refractory hypertension (HTN) even after successful treatment [2]. The current treatment guideline of a peak-to-peak blood pressure gradient (BPG_{pp}) ≤20 mmHg implemented clinically has revealed irreversible changes in arterial structure and function, yet revised guidelines have not been proposed [3]. Prior studies have been limited to older ages so the temporal evolution of mechanical stimuli at younger ages driving irreversible vascular remodeling are unknown [2]. We hypothesize that excessive coarctation-induced mechanical stimuli over time lead to changes in structure and function in the aorta and its branches, ultimately manifesting as HTN. The main objective of this work is to define specific ranges of mechanical stimuli from the severity and duration of CoA that prevent permanent remodeling (structure and function). Following IACUC approval, rabbits were exposed to BPG_{pp} severities ≤10, 11-20, and >20 mmHg for 1, 3, or 20 weeks by varying the severity and duration of CoA using permanent, dissolvable, and rapidly dissolvable sutures tied around the aorta at the sight CoA most often presents clinically. Longitudinal fluid-structure interaction (FSI) simulations over age were conducted in SimVascular (simvascular.github.io) using geometry and boundary conditions measured empirically for each group. Elastic modulus at younger ages was estimated in the simulation tuning process based on diameter variation from the systolic and diastolic phases measured during ultrasound imaging. Mechanical stimuli were then characterized including blood flow velocity patterns, medial tension, strain, and wall shear stress (WSS) indices. Preliminary data show vascular alternations such as thickening, stiffening, and dysfunction in the proximal region above the coarctation with increasing severity and/or duration of CoA. For instance, results for 20-week CoA with severity ≤10 suggest an increase in wall tension with age of ~10%, which drives changes in thickening and function. Upon quantification of mechanical stimuli from all groups, these methods will reveal the specific range of mechanical stimuli that avoid permanent vascular remodeling from CoA. The current work may then be implemented clinically via imaging and FSI modeling as part of protocols that limit the likelihood of HTN in CoA patients.

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Wall Shear Stress Estimation for 4D Flow MRI using Navier-Stokes Equation Correction

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Key Words: *phase-contrast magnetic resonance imaging, fluid dynamics, pressure field reconstruction, wall shear stress*

This study introduces a novel wall shear stress (WSS) estimation method for 4D flow magnetic resonance imaging (MRI). The method improves the WSS accuracy by using the reconstructed pressure gradient and incorporating the flow-physics constraints of the conservation of mass and linear momentum to correct the velocity gradient estimation. The method was tested on synthetic 4D flow data of analytical Womersley flow and flow in cerebral aneurysms. The proposed method's performance was compared to the state-of-the-art method based on smooth-spline fitting of the velocity profile [1] as well as the WSS calculated from uncorrected velocity gradient. The proposed method improved the WSS accuracy by as much as 100% for the Womersley flow and reduced the underestimation of mean WSS by 39% to 50% for the synthetic aneurysmal flow. The method was further applied to *in vivo* 4D flow MRI data acquired in cerebral aneurysms. The predicted mean WSS using the proposed method was 31-50% higher than predictions using the other methods. This suggested improved WSS accuracy as a previous study showed that the WSS calculated from 4D flow MRI was underestimated by 40-60% in intracranial aneurysms due to limited spatial resolution [2]. The distribution of high-WSS regions predicted using the proposed method was consistent with patient-specific CFD results. The method was further applied to *in vivo* 4D flow data in aortas. The mean systolic WSS estimated by the proposed method was 5-8 Pa, which was 4-6 times higher than the results using the other methods. The range of WSS estimated using the proposed method was consistent with the previous CFD studies, and the predicted high-WSS regions showed an improved correlation with the vortical structures (VSs) at systole. The correlation between VSs and high WSS has also been observed in a previous investigation using CFD simulations [3]. The proposed pressure-gradient-based WSS estimation method improves the accuracy of WSS estimation from 4D flow MRI data, which can help predict blood vessel remodelling and progression of cardiovascular diseases.

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Analysis of Combat Helmet Performance Integrating Blast Loading and Blunt Impact through Simulation

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Key Words: *TBI, Helmet Performance, Blast, Blunt Impact, Simulation*

The mild traumatic brain injury (mTBI) is one of the most common injuries to service members in recent conflicts. Combat helmets have been designed and evaluated to perform against ballistic and blunt impact threats, but not blast threats. An optimal design of combat helmet considering blunt, ballistic impacts and blast effects is a key requirement to improve the head protection against mTBI. Combat helmets are usually designed based on costly and time consuming laboratory tests. Computational models can offer insights in understanding the force transmission through the head-helmet system into the brain and underlying mechanism of brain injury, and help the development of effective protective design. The objective of this work is to develop a design approach integrating the effect of both blast and blunt threats to a helmet system by utilizing multi-physics computational tools and representative human head and helmet models. The high-fidelity computational models were used to capture the dynamic response of the composite shell, suspension pads, retention straps and head. We used a validated human head model to represent the warfighter's head. The helmet composite shell was represented by an orthotropic elasto-plastic material model. A strain rate dependent model was employed for pad suspension material. Available dynamic loading data was used to calibrate the material parameters. Multiple helmet system configurations subjected to blast and blunt loadings with a combination of loading magnitude and orientation were considered to quantify their influence on brain biomechanical response. Parametric studies were carried out to assess energy absorption for different suspension geometry and material morphology for different loadings. The resulting brain responses in terms of pressure, stress, strain, and strain rate as well as the head acceleration were used with published injury criteria to characterize the helmet system performance through a single metric for each threat type. Approaches to combine single-threat metrics to allow aggregating performance against multiple threats were discussed.

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A Soft-Tissue Driven Bone Remodelling Algorithm in Mandibular Residual Ridge Resorption Based on Patient CT Image Data over 5 Years

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Key Words: *Spatial Image Quantification, Soft-tissue Induced Bone Remodelling, Predictive Simulation*

Mucosa is a thin layer of nonuniform soft tissue covering bones in the oral cavity. It consists of abundant vasculature and nerve systems, acting as the gateway of material exchange to bone and providing important sensation in mastication. In the edentulous population, the residual ridge of a mandible faces significant risks of progressive and continuous bone loss, due to lack of mechanical stimulation from the missing teeth. A prosthodontic overdenture is often fitted to the mandible or maxilla to restore the masticatory function; but in the meantime, it exerts non-physiological loading to the mucosa beneath. While this thin soft issue bears and dissipates mastication forces to some extent, the compression has been found to potentially cause localised ischemia and inflammation with increasing hydrostatic pressures in the mucosa [1,2]. This ill-suited biomechanical condition is believed to accelerate this unwanted residual ridge resorption (RRR) [3]. However, the role of the biomechanical stimulation from the soft tissue has not yet been quantified or separated from the natural bone loss [4,5].

Our study recruited 8 implant-retained overdenture patients with follow-ups over 5 years, primarily aiming to elucidate the governing relationship between the RRR and the local hydrostatic pressure (σ_H) in the mucosa and then, to develop a predictive algorithm of this dynamic process. We first developed a computational framework for quantifying the localised bone profile changes to differentiate the natural and the prosthesis-induced bone loss. Patient-specific models were created from the segmented CT image sets, and the hydrostatic pressure distribution and changes in the mucosa was evaluated. The profile changes were then correlated to the local σ_H. Our results showed the total resorption under denture compression was most severe ($p < 0.001$) during the first year with an average ridge height reduction of 0.53 ± 0.08 mm. By using the resorption in the uncompressed regions as control, we found 40.6% of the resorption was induced by the compression onto the soft tissue. During the 2nd to 5th years, the total resorption gradually decreased to 0.10 ± 0.01 mm per year, and the natural bone loss was the dominant. The correlation (R^2) between RRR and the local σ_H varies between 0.55 and 0.57 with a power-law function, which has a constant term representing the natural bone loss. Based on this correlation, we can further develop a soft-tissue driven bone remodelling algorithm. In addition, our findings provide a biomechanical basis for gaining new insights into the mechanobiological responses in the soft-hard tissue interfaces to external forces, thereby benefiting the treatment.

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Computational Model Of The Bone Ecosystem During Disease

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Key Words: *Bone, Ecology, Evolution, Homeostasis, Computational*

The bone is an incredibly dynamic organ whose homeostasis emerges from the interactions between a large variety of resident cell types such as osteocytes, macrophages, mesenchymal stem cells, osteoclasts, osteoblasts, etc. These interactions are facilitated by factors and signals that help orchestrate bone dynamics. While purely experimental approaches have provided us with intriguing data and reductionistic insights, mathematical and computational models can integrate multiscale data and biological insights in ways that other models cannot. Here we use an agent-based model that captures the ecological and evolutionary features of the bone ecosystem. The models are hypothesis-driven and hypothesis-generating, they are parameterized with the help of experimental models and calibrated to capture bone's dynamic homeostasis. This model provides us with a high temporal and spatial resolution view of the bone and allows us to understand not only how it can naturally change over time but how tumors can start (or metastasize) and how the interactions between the tumor cells and the bone environment shape the Darwinian dynamics that characterize cancer progression. With the help of this model we have studied both the initiation of multiple myeloma as well as prostate cancer metastases in the bone. Extending this model to consider cancer treatments such as proteosome inhibitors (for myeloma) and androgen deprivation therapies (for prostate cancer) our model can also explain the impact of the bone ecosystem in the emergence of treatment resistance in bone cancers.

Effects of Mineralisation on Collagen Ultrastructure and Micromechanics

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Key Words: *Fibrillar network, Mineralized collagen, Turkey Leg Tendon,*

Collagen mineralisation plays a critical role in the growth, development, and ageing of tissues, including bone and its interfaces with cartilage, ligament, and tendon. One or multiple cell groups can be involved in the process, depositing mineral into the collagen matrix secreted. The soft and hard components must maintain a delicate equilibrium in order to give rise to the highly regulated and multiscale architecture, thereby meeting the biomechanical demands, such as fracture resistance [1]. Disruption of the mineralisation process is associated with many disorders like osteosclerosis, craniosynostosis, and osteogenesis imperfecta. Although extensive efforts have been dedicated to studying the mechanism of mineralisation in the intrafibrillar and interfibrillar space of collagen [2], we still have lack of understanding as to how the collagen structure changes in this process as well as the response to mechanical loading. The recent development in polarisation-resolved second harmonic generation (pSHG) microscopy revealed a hierarchical arrangement of collagen fibrillar and molecular organisation [3]. This fast-scanning label-free method allows capturing the ultrastructural features of collagen and the responses to loading.

Our study is to investigate the multiscale structural organisation and mechanical response of collagen at different degrees of mineralisation. We adopted turkey leg tendons, a widely and readily available model for studying collagen mineralisation. This avian tendon model exhibits a gradient of mineralisation in the same specimen. 4 fresh and unprocessed specimens were dissected from 20-week-old turkeys. The specimens were first imaged with x-ray absorptiometry to identify the mineralisation in the tissue. Half of the samples were individually mounted to a custom-built multiphoton microscope coupled with a tensile loading rig, on which pSHG and two-photon excitation fluorescence (TPEF) were acquired simultaneously. From pSHG data, the principal orientations and fibre dispersions of collagen were evaluated. From TPEF, the distribution and orientation of elastin were correlatively evaluated with respect to the collagen. The scans were performed under unloaded and statically loaded states at four regions of interest, namely unmineralised, fully mineralised, highly mineralised, and slightly mineralised regions. The changes in the orientation and dispersions of collagens were quantified. The other half of the specimens were scanned with x-ray diffraction on the VMXi beamline at the Diamond Light Source. This technique provides direct measurements of the orientations and anisotropy of collagen fibrils and mineral particles in specimens, as well as their changes as the responses to loading. Strong heterogeneities of collagen and elastin organisation were observed in both multiphoton and diffraction images, among and within different regions of interest along the gradient of mineralisation. The mechanical responses of the constituents will be evaluated as the next stage of this project.

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Encoding the Setpoint of Bone Functional Adaptation With Osteocytes

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Key Words: bone tissue regulation, mechanical adaptation, osteocyte, mechanostat, bone remodelling

The osteocyte network in bone is believed to play an important role for how bone tissues sense and respond to mechanical stimulation. Yet, the functional adaptation of bone is often conceptualised as a simple bone response to mechanical stimuli, such as Wolff's law or Frost's mechanostat [1], which are based on purely mechanical variables and take no account of cellular aspects of the mechanical reference state (setpoint). In this contribution, we present a theory of bone tissue sensing and adaptation based on osteocytes to provide new understanding of the role played by osteocyte signals in bone tissue regulation. This theory is based on prior work [2] and extends Frost's mechanostat theory by linking the mechanical setpoint to osteocyte properties. It further assumes that setpoint adaptation is due to the replacement of osteocytes during remodelling. We present numerical simulations to explore how mechanobiological response curves (Wolff's laws) are modulated by setpoint adaptation due to osteocyte replacement during remodelling, and by disruptions to osteocyte signals due to loss of osteocytes with age. We find that setpoint adaptation could have significant consequences, including (i) long-term irreversibility of mechanical sensitivity, which is relevant to exercise in age-related bone loss and to multi-mission astronauts; and (ii) hysteresis in Wolff's laws, which may be experimentally observable.

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Fatigue analysis of reconstruction plate by considering time-dependent bone remodelling

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Key Words: *XFEM, Fatigue fracture, Bone remodelling, Mandibular reconstruction plate*

Large mandibular defects resulted from trauma, tumour, or osteoradionecrosis represents some common and critical morbidity in the maxillofacial reconstruction. Using osteosynthesis devices to bridge the defect with fibula free flap (FFF) has become a major approach for mandibular reconstruction, owing to the advantages of adequate bone length, low donor site damage, and an abundant periosteal blood supply[1]. However, failure of these devices due to fatigue under cyclic loading has been recognized as a primary concern on therapeutic longevity. In this study, we develop a computational approach for modelling fatigue process in the reconstruction plate based upon the eXtended Finite Element Method (XFEM). When a reconstruction plate is placed, the bone would remodel itself continuously; thus, the stiffness of the prosthetic system would change over time [2] The crack initiation and propagation due to the excessive loads will affect the stiffness of the plate and consequently bone remodelling process by varying the mechanical loading transfer on the bone. To investigate the interaction between fatigue process and bone remodelling, we propose a time-dependent fatigue analysis approach by taking into account the effect of the Wolff's law-based bone remodelling process. The influence of biting force measured over treatment time on the fatigue life of fixation plate and bone remodelling is also analysed. Under various occlusal loadings, the interactive effects between fatigue crack growth and bone remodelling are investigated to obtain some new insights into the design of prosthetic devices. This study showcases an effective approach for predicting fatigue failure of prosthetic devices *in-silico*, thereby guiding design optimisation of patient-specific prosthetic devices to ensure their longevity.

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Geometric Control of Bone Tissue Growth: Analysing Asymmetric Osteons

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Key Words: bone tissue regulation, mechanical adaptation, osteocyte, mechanostat, bone remodelling

Osteonal pores in cortical bone provide highly confined spaces infilled by new bone during bone remodelling. The geometric crowding and spreading of new tissue material at concave and convex areas of the bone surface induce strong geometric control on the rate of growth of new bone tissue in these pores. A record of the differential growth rates is provided by the concentric rings of lamellae seen in the new bone. The lamellae indicate past surface locations, and their arrangement and geometry give insights into bone generation mechanisms [1]. However, these experimental data comprise a tangled combination of geometric influences and cell behavioural influences of bone tissue growth.

To disentangle these influences, we build on a mathematical model of the geometric control of cells growing new tissue, based on rigorous principles of material balance on moving boundaries [2]. The mathematical model enables us to factor out the mechanistic influence of geometric crowding on growth rate in the experimental data. By comparing numerical simulations of pore infilling with experimental osteon geometries quantitatively, we gain insights into the diffusive and active/inactive behaviours of the cells in a variety of regular and irregular osteonal pores.

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Nanoindentation Protocol for Identifying Elasticity of Periodontal Ligament

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Key Words: *Nanoindentation, Periodontal ligament, Mechanical properties, Soft tissues*

The load bearing integrity of tooth against chewing stresses within alveolar bone is most likely associated with instantaneous stiffness and subsequent time-dependent stress relaxation of periodontal ligament (PDL). Despite it comprising only thin (hundreds of microns) outer membrane of tooth root, PDL characteristics meet the multifunctional criterial, hence identifying the mechanical properties of PDL is an important insight to conceptualize new load bearing biomaterials and/or industrial applications. A major difficulty of this concept is lack of precise first-hand data of PDL at tissue level. Here we demonstrate a new nanoindentation protocol for PDL and its validations.

This study adopted 7-week-old male BALB/c mice as the animal subject and euthanized it in a carbon dioxide chamber. Immediately after the sacrifice of the animal, the hemi-mandible, containing three molars and one incisor, was excised and dissected at the fibrous mandibular symphysis. All the animal procedures in this study were developed in accordance with Guiding Principles for the care and use of Animals.These specimens were transversely cross sectioned using a microtome at the level of cervical line as well as the approximately mid-root level of the molars, exposing the PDL at different anatomical position for nanoindentations.

Nanoindentation tests were carried out using a quantitative nanomechanical test instrument (TI 950 TriboIndenter, Hysitron, Inc, Eden Prairie, MN, USA). A diamond flat-end indenter with 10 μm diameter was used for corresponding to required measurement size for fiber bundles. The indenter was attached to the high bandwidth transducer (nanoDMA III, Hysitron Inc.) allowing dynamic mechanical analysis (DMA) on PDL. The load applied to the PDL was controlled using a feedback closed-loop load-control algorithm for all the tests. Force-displacement curves were recorded under loading rates of 10 μN/s with a maximum force at 50 μN. The loading portion was followed by 2 sec holding with superimposed dynamic oscillations at a frequency of 200 Hz and displacement amplitude of 1-2 nm. The dynamic sinusoidal oscillation captures contact (storage) stiffness almost associated with loading strain so that storage moduli were measurable. A validation was also carried out using a quasi-static load function, using the fast loading/unloading rate (50 μN/0.1s) so that elastic and viscoelastic responses can be discerned, since viscus portion cannot be responsible against such fast loading/unloading strains.

Both calculated storage moduli and quasi-static elastic moduli were comparable, hence instantaneous elastic modulus of PDL at fiber bundle level is around 100 MPa irrespective of loading rates. Further investigation of delayed viscoelastic response with a combination of FEA and first-hand nanoindentation data would be desirable to fully understand the nature of PDL.

Regional Variations in Articular Cartilage Ultrastructure and Micromechanics

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Key Words: *Articular cartilage, regional variations, micromechanics, pSHG,*

Central to the functions in load bearing and mobility, the biomechanical properties of articular cartilage arise due to its extracellular matrix (ECM) consisting of a collagenous network interacting with an interstitial fluid rich in proteoglycans [1]. The recent development in analysing the polarisation-dependence of second-harmonic generation (pSHG) imaging revealed hierarchical complexities of collagen fibrillar and intrafibrillar organisation [2, 3]. This advance technique allows examination of the well-known zonal variations along with the depth of the tissue across length scales. The fast-scanning speed also provides capability of visualising dynamic responses to external loading, to which both levels of structural organisation were found highly sensitive. However, a quantitative relationship between the collagen organisation and the mechanical response has not yet been established. Apart from the zonal variation, different compartments and regions of the joint experience different types of mechanical loading [4]. We hypothesize that the collagen organisation is tailored to its local biomechanical environment at different anatomical locations of the joint, and such organisational variation is also manifested in their susceptibility to injury and degenerative disease, like osteoarthritis.

The overarching aim of our study is to establish a quantitative relationship between the cartilage structural organisation and its biomechanical function by comparing different regions of articular joints. A pair of bovine metacarpophalangeal (MCP) joints were acquired from a local abattoir, and 24 explants in cuboid shapes were harvested from the medial, lateral, and patella-femoral compartments. We first map the longitudinal cross-section of the explants with pSHG and evaluated the structural variations among three zones (superficial, transitional, and deep zones) by quantifying the principal angles and degrees of dispersion of collagen. Next, the same specimens were mounted and loaded on a custom-built rig integrated with our pSHG microscope, to visualise structural responses under two levels of tissue strains applied at 8% and 16%. These two strain levels present a medium and an extreme case in normal activities, respectively. The structural responses were evaluated in terms of the re-orientation and re-alignment of the collagen fibrils.

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A numerical study on the generic flexible-cell focus in viscoelastic flows

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Key Words: Immersed boundary method, fluid-structure interaction, viscoelastic flow

The generic flexible-cell focus in viscoelastic flows through a contraction-expansion microchannel is investigated by an immersed boundary-lattice Boltzmann method [1, 2]. The effects of the fluid viscoelasticity, the initial position of the cell and the confinement of the microchannel on the cell migration are evaluated. It is found that the migration of the cell includes two stages: (a) the migration in the center plain and (b) the migration away from the center plain. At stage (a), the cell may focus to one trajectory or different trajectories (from different initial positions) depending on the viscoelasticity of the fluid and the confinement of the microchannel. The viscoelasticity of the fluid and the confinement of the microchannel facilitate the focusing of the cell. At stage (b), the cell focuses to a steady trajectory after a long-term migration. The equilibrium projected trajectory of the cell (on a cross section of the microchannel) forms a ring, and the stronger viscoelasticity of the fluid generally induces a higher equilibrium trajectory of the cell.

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Agent-Based Models of Biophysical Interactions in Multicellular Systems

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Key Words: Agent-Based Model, Open Source, Multiscale, Multicellular Systems, PhysiCell

Multicellular systems–ranging from ecosystems of single-cell organisms to healthy and diseased tissues–are dynamical multiscale systems where complexity emerges from myraid cell-cell and cell-environment interactions. Cells can read chemical and mechanical signals in their environment, and process them via complex intracellular networks to drive changes in their metabolism, proliferation, death, migration, mechanical characteristics, and secretion of chemical signals to communicate with other cells [1]. Chemical and mechanical signals can propagate through over fast time scales across short distances (e.g., by contact), or over slow time scales over larger distances (e.g., by diffusion). Simulation models can act as "virtual laboratories" to help understand these highly nonlinear systems, but cellular-scale heterogeneity and stochasticity sometimes require that such models incorporate cell-scale behaviors and interactions.

After introducing cell-based models [2], we will describe PhysiCell [3]: an open source, cross-platform 3-D simulation platform that models individual cells as discrete agents in complex chemical microenvironments governed by reaction-diffusion equations. We will describe general formulations for cell-cell interactions by contact, mechanics, and chemical communication. Using this repertoire of interactions, we will explore a broad range of models including mechanics-driven arrest of cancer metastases [4], hypoxia-driven cancer invasion [5], predator-prey systems, oscillations in cell colonies, cell specialization, cancer-immune interactions [6], and multiscale modeling of immune response to viral infections [7]. We will also describe how PhysiCell can be combined with intracellular signaling models into multiscale models that span from molecular to tissue scales [8]. We will conclude by demonstrating recent advances to create a simplified "signal-response" representation of cell-cell interactions, and to use this to create graphical "expert-in-the-loop" model design tools for multidisciplinary teams.

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Computational Investigation of Cell Shape Changes Driven by Actomyosin Contractility

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Key Words: *Actin, Myosin, Bleb, Cell, Actomyosin contractility*

Changes in cell shapes are mostly driven by forces generated from the cytoskeleton. Recently, several in vitro experiments developed a synthetic cell-like system consisting of actin networks, cross-linking proteins, and myosin motors encapsulated by lipid vesicles or water droplets in order to study cell-scale behaviors facilitated by forces generated from actomyosin networks. However, these experiments are very hard to conduct, thus preventing exploration of wide parametric spaces. To overcome experimental limits and thus perform extensive parametric studies, we developed a novel agent-based model for a minimal cell-like structure comprised of discrete actomyosin cortex, osmotic pressure, and cell membrane simplified into a triangulated mesh. The cortex is coupled to the cell membrane to various extents via cross-linking proteins. Using this model, we found how cell shapes are regulated by a competition between actomyosin contractility that tends to induce contraction and osmotic pressure that tends to lead to expansion. We demonstrated that bulge that mimics cell blebs can be formed when the coupling level between the cortex and the membrane is intermediate. Our results provide insights into understanding how cell shapes are regulated under diverse conditions.

Computational Modeling of Pressure-Driven Cell Motility under Confinement

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Key Words: *Cell mechanics, Fluid-structure interaction, Regularized Stokeslets*

Cell migration is critical for many vital processes, such as embryogenesis and tissue repair, as well as harmful processes, such as cancer cell metastasis. In experiments, cells have been shown to exhibit different migration strategies based on the properties of their external environment [1]. For example, cells migrating through a 3D gel use myosin-driven rear contraction for motility [2]. In [3], cells migrate using round membrane protrusions called blebs while confined between two surfaces, a gel and glass coverslip. Additionally, recent experiments demonstrate that cells do not need to adhere to the channel walls in order to migrate under confinement [4], yet it is unclear how traction forces are coordinated in space and time to generate motion. Dynamic 2D computational models of a migrating cell using intracellular pressure gradients generated by (1) rear contraction and (2) blebbing in a narrow channel are presented. The cell model consists of an elastic membrane, poro-(visco)elastic cortex, membrane-cortex adhesion, and the fluid cytoplasm. Evolution equations for the actin density of the cortex are included for modeling bleb retraction. The channel walls are modelled as rigid structures with different shapes. The model is formulated using the method of regularized Stokeslets [5]. Results show that the cell cannot effectively migrate when the cortex is modeled as a poroelastic structure using repeated cycles of either rear contraction or blebbing, even when the channel walls are asymmetric. Simulation data show cells can migrate in symmetric and asymmetric straight channel walls only if the cortical turnover is included by modelling the cortex as a poro-viscoelastic structure.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Fluid-structure interaction simulations of blood cells and the endothelial surface layer

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Key Words: Fluid-structure interaction, Blood cell motion, Wall-induced migration

Many fluid-structure interactions in biology involve the near-contact of elastic objects separated by a thin layer of viscous fluid. In viscous fluids such as blood, deformable objects can acquire lift forces and migrate away from walls, a phenomenon known as wall-induced migration [1].

Blood vessels are lined by an endothelial surface layer that has a thickness up to 1 micron. This layer has physiological roles in fluid-solute exchange and coagulation response, and may also influence blood flow through interactions with the suspended blood cells [2].

To simulate the interaction of red blood cells with vessel walls, we use the immersed boundary method [3] to explore the effects on red blood cell lift of surface roughness and changes in the endothelial surface layer thickness that arise in pathological conditions such as sepsis. Perturbations in the lift force lead to changes in the cell free layer, which we speculate may have consequences on the spatial distribution of platelets, which indicates potential importance of the endothelial surface layer.

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Microscale flow dynamics of blood cells in health and disease

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Key Words: *Red blood cells, Blood disorder, Flow dynamics, Multiscale modelling*

In humans, normal red blood cells (RBCs) are flexible and deformable. The extreme deformability allows them to squeeze through narrow capillaries without any damage. However, in many blood disorders, the membrane defects of diseased RBCs cause the impaired blood flow and other pathophysiological aspects of disease-related vascular complications. By combining dynamic microfluidic experiments with multiscale simulations, we investigated the biomechanical properties and flow dynamics of RBCs in health and disease. We showed that the RBC undergoes a severe deformation as it traverse microvascular passages, and the membrane defects of the RBCs play a crucial role in the regulation of blood flow.

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Modeling and Simulation of Osteocyte-Fluid Interaction

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Key Words: *Osteocyte, Mathematical Modelling, Lattice Boltzmann, Immersed Boundary*

The osteocyte is a bone cell that is responsible for mechanotransduction and guides growth and remodeling in bone. The cell consists of a nucleus, cytoskeleton, cytoplasm, plasma membrane, and numerous dendritic cellular processes. It is encased in a lacuna in the lacunar-canalicular network that permeates the bone matrix. The interstices between the cell and the bone matrix are filled with a salt-water-like fluid and the pericellular matrix (PCM), which consists of cell-associated proteins surrounding the cell. When the bone is mechanically loaded, the interstitial fluid is forced through the PCM, introducing stresses on the cell. Experiments suggest that those stresses and associated strains are amplified approximately ten-fold compared to the macroscale stress and strain that occur during normal motion. The mechanism of this stress amplification is not well characterized. *In vivo* experiments are challenging to conduct because of the complexity of the osteocyte's microenvironment. Modeling and simulation, however, can provide a viable approach for shedding insights into the force amplification that occurs in the system.

Here, we use two mathematical models to characterize the force amplification mechanism in osteocytes. In the first two-dimensional model, the osteocyte's main body is modeled as a deformable ellipse composed of multiple interconnecting flexible fibers, which represent the membrane and the internal cytoskeleton, immersed in viscous flow, representing the cell's cytoplasm/interior. The cellular processes are modeled as multiple flexible fibers attached to the main body that are immersed in a viscous incompressible fluid that represents the surrounding interstitial fluid of the lacunar-canalicular network. That fluid is encased in the bone matrix that is modeled as a rigid body whose wall bounds the fluid region. To approximate typical motion, a random set of canaliculi are modeled as outlets while the remaining canaliculi are modeled as inlets. We consider the influence of the number and geometry of the canaliculi on the wall shear and normal stress on the osteocyte membrane and processes. The second three-dimensional model is based on images taken during laboratory experiments. The osteocyte is represented as a network of connected tetrahedrons immersed in a viscous incompressible fluid, with different refinement levels for the membrane, cytoskeleton, and nucleus. Each tetrahedral edge is made of a deformable fiber. The model considers how stress and strain are distributed throughout the osteocyte's main body when external flow exerts force on the cell. In both models, the viscous flow is modeled by the lattice Boltzmann equations (D2Q9 and D3Q19) and the fluid-structure interaction is modeled by the immersed boundary method.

Numerical simulation of active surface dynamics leading to cell division and migration

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Key Words: *Active surface, Free-boundary problem, surface-bulk coupling, viscoelastic surface, cell shape dynamics*

Mechanochemical processes play a crucial role during morphogenesis, the formation of complex shapes and tissues out of a single cell. On the cellular level, the actomyosin cortex governs shape and shape changes. This thin layer of active material underneath the cell surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules. Advective transport of such molecules leads to a complex interplay of hydrodynamics and molecule concentration which gives rise to pattern formation and self-organized shape dynamics [1,2].
In this talk, we present a numerical model to simulate an active surface immersed in viscous fluids. The cortex is modelled as a viscoelastic surface material [3], described by a freely evolving Finite-Element grid. The dynamics are coupled to a surface concentration equation of force-generating molecules (actomyosin).
We show the resulting mechanochemical patterns which emerge in different parameter configurations. This patterning goes along with surface and intracellular flows which drive cell division or cell migration, accompanied by impressive cell shape dynamics. We compare the results to linear stability analysis [2] and experimental data.

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On a Finite Strain Modeling of Yeast Cell Growth Stimulated by Turgor Pressure

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Key Words: Cell-wall, Saccharomyces cerevisiae, Growth, Turgor pressure, Large deformations

Growth is a phenomenon that occurs in almost all living cells. It is essential for important cellular events such as organism development and cell division. In particular, *Saccharomyces cerevisiae* yeast has been one of the preferred organisms for the study of growth [1]. Yeast cells polarize their growth in response to both external and internal stimuli. In the present study, focus is made on internal ones. Being walled cells, they possess high internal turgor pressure that allows them to grow and survive in the environment.

A theoretical and numerical modeling is derived to describe this growth. Yeasts are herein regarded as axisymmetrical shells and, in view of their soft nature, a finite strain approcah is adopted. The kinematical choice is based on the multiplicative decomposition of the deformation gradient into an elastic part and growth part. It is shown how continuum thermodynamics is crucial in setting convenient forms for the coupling between stress and growth, e.g. [2]. As a modeling example, an Ogden-type constitutive relation is used for the elastic part, and for the growth evolution, a potential is introduced that takes into account the stress stimulation through a growth threshold and a characteristic time parameters.

The whole framework is embedded into a finite element context. For the shell kinematics, use is made of the quasi-Kirchhoff type theory for thin shells of revolution derived in, e.g. [3]. In this case, the meridional and circumferential strains are regarded as principal. Hence, this allows for an easy use of a theory based on principal stretches of the Ogden-type. Representative numerical simulations are given that show, among others, the influence of the turgor pressure as a stimulus for growth, and the influence of the characteristic time for its kinetics.

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Phase-Field Model of Vesicle Motion and Deformation and Its Computation

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Key Words: *Multiphysics Problems, phase-field modeling*

A thermodynamically consistent phase-field model is introduced for simulating motion and shape transformation of vesicles under flow conditions. In particular, a general slip boundary condition is used to describe the interaction between vesicles and the wall of the fluid domain. A second-order accurate in both space and time C0 finite element method is proposed to solve the model governing equations. Various numerical tests confirm the convergence, energy stability, and conservation of mass and surface area of cells of the proposed scheme. Vesicles with different mechanical properties are also used to explain the pathological risk for patients with sickle cell disease.

The Effects of Vessel Wall Proteins on Red Blood Cell Dynamics at Diverging Vessel Bifurcations

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Key Words: *Bifurcation, Endothelial surface layer, Red blood cell mechanics, Capillary flow*

Experiments have shown that red blood cells (RBCs) are nonuniformly distributed throughout the microvasculature. With RBCs making up approximately forty to forty-five percent of blood, this has important consequences for transport of materials such as oxygen (carried by RBCs), nutrients, other cells, and drugs. In nonuniform partitioning at diverging vessel bifurcations, where blood flows from one vessel into two downstream vessel branches, downstream branches with higher percentage flow regularly claim an even higher percentage of RBCs in that branch. This phenomenon plays a significant role in the earlier mentioned nonuniform distribution of RBCs throughout the microvasculature.

While many studies have considered different aspects of partitioning, few have considered the effects of a protein layer that coats the vessel wall often referred to as the endothelial glycocalyx layer, glycocalyx, and/or endothelial surface layer (ESL). The ESL has been increasingly recognized as being important with identification of its role in overall vessel flow resistance and in general cell adhesion to vessel walls. Despite this increasing recognition, studies have not yet explicitly targeted the potential effects of this important layer on RBC dynamics during partitioning.

To better understand how the ESL may affect partitioning, we constructed a computational model of RBCs passing one at a time through a bifurcation lined with a 1 micron thick ESL. RBCs are represented by an interconnected set of damped springs. The surrounding fluid is modelled using the Stokes flow equations. The ESL is modelled as a porous media that resists compression. The system is solved using a finite element solver that couples the three systems together. Decreasing the ESL's hydraulic resistivity and/or its resistance to compression generated more nonuniform partitioning. We also considered how ESL properties affected RBC deformation and penetration of the ESL. We found that decreasing the ESL's hydraulic resistivity and/or its resistance to compression increased RBC penetration of the ESL and, usually, decreased RBC deformation. We will also share preliminary results on how varying ESL properties affect RBC interactions with each other as they pass through a bifurcation. While all results are limited to very low hematocrits and a somewhat specific setting, they provide a strong start towards more fully characterizing ESL-RBC interactions including effects on RBC deformation dependent activity such as release of vasodilators and on RBC adhesion assisted clotting.

A Novel Chemo-Mechano-Biological Model of Osteoarthritic Cartilage

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Key Words: *articular cartilage, mechanobiology, growth and remodeling, mathematical model*

Nearly 20% of people in the US suffer from osteoarthritis (OA) affecting the quality of life through pain, functional limitations, lost earnings, anxiety, and depression – yet we still do not understand the cause nor progression of the disease. While mechanical stimuli helps to maintain the healthy status of cartilage, overloading (e.g., trauma) and reduced loading (e.g., immobilization) causes upregulation of catabolic cytokines and downregulation of anabolic growth factors resulting in morphological and mechanical changes (e.g., softening, fibrillation, ulceration, and erosion). Current investigations of the effects of mechanical loading on cartilage – including both *in vitro* experiments with human cartilage and *in vivo* animal models – fall short of true human physiological relevance. Current mathematical models of signalling pathways lack mechanical inputs, while the biomechanical models lack the effects of cytokines. Here we propose a novel chemo-mechano-biological mathematical model including anisotropic, volumetric changes affecting the load-bearing behavior of osteoarthritic cartilage.

Leveraging our constitutive model for cartilage [1] we establish evolution equations for key chemical species and solid constituents [2], whereby the progression of OA results in volume loss normal to the articular surface [3]. We simulate six physically relevant conditions in the knee over 30 months: both normal walking and immobilization in health or after injury, and two therapeutic interventions after injury. Our model predicts homeostasis (i.e., no changes in the constituents or cytokines) for healthy individuals walking normally. Immobilization of healthy individuals increases both cytokines and loss of mass/volume of key constituents. The adverse effects of injury improve with normal walking but worsen with immobilization. Therapeutic interventions produce improvements in the mass of key constituents. Our proposed framework is a first step towards a new class of computational tools that consider, for the first time, the turnover and production of constituents and cytokines within cartilage in health and disease.

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Adaptive finite element *in silico* modelling of cartilage mechanobiology bridges the *in vitro* and *in vivo* approaches in osteoarthritis research

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Key Words: *Articular Cartilage, In silico Modelling, Finite Element Analysis, Mechanobiology*

Osteoarthritis (OA) is a multifactorial disease characterized by cartilage degeneration [1]. *In vitro* and *in vivo* animal experiments show that altered mechanical loading is a driver of OA onset and progression [2, 3]. However, a thorough understanding of the mechanisms behind cartilage degenerative changes and their interactions in healthy and OA cartilage remains to be further elucidated.

In the "Happy Joints" project we use *in silico* modelling as a bridge between *in vitro* and *in vivo* experiments investigating the role of mechanical loading on cartilage homeostasis. Our musculoskeletal computational models can estimate realistic mechanical stimuli as seen in the joint, as well as validate and optimize parameters used in *in vitro* and *in vivo* experimental designs. We implement cartilage mechano-regulatory algorithms reflecting healthy and OA cartilage biology in *in silico* models through adaptive finite element approaches [4]. These models relate the mechanical loading on cartilage to tissue degeneration and regeneration based on observations from *in vitro* bioreactor experiments and biological analysis. After calibration and validation with experimental data, the adaptive finite element models can predict cartilage tissue adaptation upon mechanical loading. Our adaptive modelling results show that collagen fibril degradation has a unique role in OA progression followed by injurious mechanical loading, as it contributes to developing a cartilage tissue degeneration loop once the collagen degradation has been started.

This work relies on a multidisciplinary approach combining expertise from biology, tissue engineering, computational, biomechanical and clinical fields, in a new interdisciplinary research line called "mechanomics". In the short term, our computational models can help reduce *in vitro* experiments and contribute to the 3Rs in animal research (replacement, reduction, refinement). In the long term, validated models of cartilage mechano-regulation in humans have the potential to be translated into a clinical setting to predict cartilage adaptation after interventions, such as tissue engineering approaches, surgery, exercise and drugs.

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An *in-silico* approach to quantify apoptotic effects of cold plasma jet and cytotoxic drug on murine melanoma cancer cells

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Key Words: *Cold plasma jet, Cytotoxic drug, Melanoma, In-silico, Agent-based model*

Atmospheric Pressure Plasma Jet (APPJ) is very promising in such that it can effectively be used against cancer. Plasma jet produces reactive species, ultra-violet radiation, and intense electric fields, which affect the functionality of biological matter, avoiding thermal damage due to the low APPJ gas temperature [1]. In various *in-vitro* and *in-vivo* studies, APPJ are applied either directly (i.e., cancer cells cultured in media subjected to APPJ) or indirectly (i.e., APPJ-treated cell media injected to cancers). Furthermore, APPJ can be used as adjuvant therapies with other cancer treatment modalities to achieve enhanced therapeutic outcomes [2]. To date, very few research works have investigated APPJ effect on neoplasia using *in-silico* models.

In this work we present a novel *in-silico* model to simulate murine melanoma cancer cell response to helium APPJ or/and doxorubicin drug (DOX). The *in-silico* considers an agent-based modelling approach [3]. The model is informed by relevant *in-vitro* experiments on cancer-cell viability that provide information on cell number development during incubation, and probability values for apoptosis and mitosis following subjection to a plasma-conditioned medium, DOX, and DOX combined with APPJ. The simulations highlight the impact on cell number, apoptosis or/and mitosis of each treatment scenario, depending on plasma-treatment duration and DOX concentration. The *in-silico* results agree with the corresponding *in-vitro* data. The proposed modelling approach offers great potential to predicting cancer-cell behaviour upon exposure to APPJ or/and chemotherapeutics by quantifying cell biomechanics – this demonstrates the capacity of *in-silico* in plasma (cancer) medicine.

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Applying 3-D Computational Homogenization to Model Collagen Microdamage in Cartilage

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Key Words: *articular cartilage, theory of porous media, FE^2 methods, microdamage*

While microcracks in bone have been characterized extensively, and sub-millimeter-scale surface fissures are well known for early to advanced osteoarthritis (OA), we recently demonstrated that low-energy impact usually considered non-injurious can in fact cause micrometer-scale cracks in the collagen network of human cartilage [1]. While pre-clinical OA may originate with microcracks in the network of collagen, it is likely crack propagation in the extracellular matrix (ECM) that initiates the cascade of OA degeneration. However, the extent of microcrack propagation during repetitive mechanical loads to cartilage during normal daily activities is unknown. Finite element (FE) models are well-established at the macro (e.g. joint) scale, but accurate intra-tissue modeling must reflect complex intra-tissue interactions. Emerging multi-scale FE^2 methods (FE analyses augmented to derive the material behaviors from a distribution of finer scale FE analyses) are ideally suited to bridge the joint and intra-tissue scales, but have not yet been applied to multi-phase fibrous cartilage. We combined the theory of porous media (TPM) [2] and the FE^2-method [3] (i.e. the TPM^2 method) to solve 3-D, two-scale, non-linear, coupled, and time-dependent boundary value problems for materials with porous microstructures. We simulate, using our custom TPM^2 modeling framework implemented in FEBio, unconfined compression of cartilage explants. Within the superficial zone we employ new fibrous RVEs (with microcracks initiated) while the remaining cartilage (middle and deep zones) uses our existing custom FE framework. We perform: (1) sensitivity analysis on the modeling framework to quantify prediction sensitivity to input material parameters, (2) statistical analysis of material parameters to determine patient-dependent ranges. Finally, validation studies using cartilage explants to quantify propagation of microcracks ex vivo will confirm the predictive power of the simulation tools for ex vivo and in vivo studies [4]. The TPM^2 framework we established to understand how physical activity propagates microcracks in the collagen network of cartilage not only characterizes one of the earliest observable signs of deterioration related to osteoarthritis (OA), but also facilitate studies of other soft tissues and engineering materials.

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Effect of Hardware Density Reduction to Avoid Proximal Junction Failure in Adult Spine Surgery: FE Analysis

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Key Words: *Proximal Junction Failure, Finite Element Model, Adult Spine Deformity*

Purpose: Post-operative incidence of Proximal Junctional Failure (PJF) is observed by 61.7% in sagittal imbalance surgery [1]. In this study, Finite Element Model (FEM) is employed to find out the biomechanical etiology of PJF, highlighting effect of hardware density reduction.

Material and Methods: In this study, 42 patients (20 controls and 22 failures, EOS modality) are selected using inclusion criteria: age 50-75, Pelvic inclination> 20°, SVA> 5cm, PJF complications by the Hart criteria [2]. 3D spine tetrahedral meshes for non-operated images are generated using sterEOS software. To deploy the Statistical Shape Model (SSM), all 3D models are aligned and using Principal Component Analysis (PCA), principal modes of variation are obtained. Unstructured meshes of mean model is converted to the structured meshes using morphing techniques (TPS [3] for vertebras, and CPD [4] for IVDs). Then, dense deformation fields of SSM are applied to the mean structured model in order to have robust structured SSM. Two P-S control and failure models are regenerated including ligaments. Anisotropic hyper-elastic [5], linear elastic [6] and hypo-elastic [7] models are introduced for material properties of IVD, vertebra and ligaments, respectively. Eccentric load path in each vertebra centre is applied based on the weight of the patient [8]. Following FE simulation steps are used: 1-8hrs pre-swelling for IVDs, 2- 15mins to apply kinematic constraints (deformation fields between pre-op and post-op model) to correct the spine, 3- 1min for Instrument implantation and applying eccentric loads and 4- 3hrs to have steady-state conditions.

Results: Two P-S control and failure cases with hardware extended to T10 (UIV) are compared using FEM. Results revealed that the fibre maximum principal strain in IVD of UIV/UIV+1 in the failure case was 73.99% higher than in the control case (16.06% vs 9.23%). Also reducing 2 or 3 screw level below the UIV in the failure case could lead to get closer the mean fibre strain to the control. However, screw pull-out force was increased by 54% in case of hardware density reduction. But use of Cr-Co rod instead of TiAl4V could decrease pull-out forces by 50.5%.

Conclusions: Increasing fibre strains at UIV/UIV+1 may cause incremental disc degeneration in the etiology of PJK and leading to PJF. Also, screw density reduction reduces the chronic load at proximal IVD. However, such reduction has a limit because of screw pull-out. Trade-off analyses showed that removing 2 screws inferior the UIV with Cr-Co rod would be optimal by controlling the IVD strain and screw pull-out force. Effect of osteoporotic is interested for future works.

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In Vivo Cartilage Elastography Determines Mechanical Properties from Dynamic MRI

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Key Words: *articular cartilage, inverse modelling, MRI, mechanical properties*

Osteoarthritis (OA) is a degenerative joint disease that is a leading cause of joint pain, disability, and health care costs worldwide. Diagnosing early-stage OA can be difficult due to a lack of validated outcome measures for individuals with early knee OA [1]. As most OA progresses from an initial injury to the superficial zone of cartilage and leads to biochemical and mechanical changes to the entire cartilage region, quantifying changes to cartilage material properties non-invasively in vivo is of substantial interest. MRI is unique among imaging tools as it can characterize tissues with high spatial detail, has a deep penetration depth, and can assess tissues noninvasively [1]. Recently, displacement encoded stimulated echo MRI (DENSE) has been used to calculate pixel level full field displacement maps of soft tissues under repetitive motion [2]. Leveraging this previous work, here we coupled DENSE MRI to displacement under applied loading MRI (dualMRI) to capture in vivo full field displacement and mechanical strain maps of the human knee while under load. We then present data for animal and human subjects combining this MRI method and a novel post-processing pipeline to acquire full-field cartilage displacements, and quantify *in vivo* cartilage stiffness and Poisson ratio.

An MRI-compatible loading apparatus that provides a varus-valgus load along the joint line of the knee was manufactured and validated. Following validation, the subject was imaged in a clinical MRI system (3T; Siemens Prismafit) using a cyclic loading regime (pneumatic, 25N load at foot, 1s load, 1s unload) to mimic a walking cadence. DENSE MRI was collected following achievement of quasi-steady-state response within the cartilage. Displacements for each pixel within the cartilage ROIs were determined and smoothed from phase data using custom software [2]. Material property characterization leveraging full-field displacement information was accomplished by combining both the virtual fields method (VFM) and a constrained FEBio-based optimization method to determine medial cartilage material properties. Ultimately, we hope this framework can provide a way forward to measure cartilage material properties in a clinical MRI setting and could potentially be extended to other load-bearing musculoskeletal tissues, including ligament and intervertebral disc.

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Mechanotransduction computational approach of chondrocytes

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Key Words: *Chondrocyte, Mechanotransduction, Network modelling, Osteoarthritis*

Osteoarthritis (OA) is a debilitating joint disease, characterized by articular cartilage degradation, local inflammation, and pain. An extensive range of *in vivo* and *in vitro* studies provide evidence that mechanical loads induce changes in chondrocyte gene expression, through a process known as mechanotransduction (MT). MT involves cascades of complex molecular interactions that, when triggered, convert physical signs to cellular response(s) that favor chondroprotection or cartilage destruction regarding the nature of loads. Systematic representations of those interactions can positively inform early strategies for OA management, and dynamic modelling allows semi-quantitative representations of the steady states (SS) of the system according to imposed initial conditions. In cell biology, we would compare long-term cell activity or phenotypes to these SS or attractors. To this end, a novel network-based model (NBM) in the form of a continuous dynamical system of CC activity is proposed.

The NBM incorporates key interactions from a corpus of 82 peer-reviewed articles from indexed journals. Then, an interactome is developed, consisting of a set of 115 nodes, i.e., cellular receptors, second messengers, transcription factors and proteins, related to each other through a specific topology of 256 directed edges. It is converted into a semi-quantitative mathematical model through a system of differential equations. To simulate a healthy SS of a CC including MT, the network is first stimulated with a physio-osmotic initial condition (TRPV4 and $(\alpha_5\beta_1$ activation). We further assess its capability to predict expected SS under inflammation and injurious loads (under static compression (ST) or high hydrostatic compression (HC) when PIEZO channels and patched receptor (PTCH) become activated). To validate the model, a qualitative validation (QV) is performed: we look for reported experiments and then we have counted how many of them can be replicated with our NBM.

Results show that under physio-osmotic conditions, an anabolic SS is reached with low levels of matrix metalloproteinases (MMPs), and high levels of structural proteins. Pro-inflammatory and HC perturbations lead to a significantly different (t-test, α=0.05) CC expression profile, as a catabolic SS is reached, reflected by fully expressed pro-inflammatory cytokines and MMPs. ST does not have such a strong influence on chondrocyte metabolism, but it reduces the presence of anabolic indicators. Regarding transcription factors, healthy markers (Sox9 and CITED 2) are fully expressed under physio-osmotic conditions, and reduced under inflammation, HC and ST. Contrary, NF-kB and Runx2, characteristic of an osteoarthritic CC, are activated by inflammation, HC, and ST. Concerning the QV, our NBM can replicate 88% of the experiments tested, but PTCH related experiments could not be reproduced, suggesting the need for a targeted enrichment of the NBM.

A regulatory network that maps intracellular signalling pathways of a CC was successfully developed. The model could predict expected MT and inflammation effects on general cell metabolism, revealing the potential of exploitation in OA.

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Modelling Regenerative Angiogenesis to Inform Peripheral Nerve Repair Construct Designs

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Keywords: Discrete-Continuous Model, Multiphysics, Multiscale, Angiogenesis.

Peripheral Nerve Injuries (PNIs), affect more than 1M people per year in Europe and the USA [1] with estimated costs above £1B in the USA alone. Paralysis and loss of sensation are common in severe PNIs, potentially leading to lifelong pain and loss of autonomy for patients. The current gold-standard treatment for large-gap PNIs use autografts to bridge between severed nerve stumps. Such a treatment requires additional surgeries, induces donor-site morbidity, and often yields underwhelming functional recovery [2].

Engineered Neural Tissue (EngNT) [3] is being developed to address these issues. EngNT constructs consist of cylindrical cellular hydrogels surrounded by a sheath of protective material. They aim at providing a supportive microenvironment to accelerate regeneration, whilst also enabling the careful spatial seeding of therapeutic cells and other regenerative factors.

Revascularisation of the injury site is an essential preliminary step of nerve repair, as microvessels are central in the delivery of nutrients and can serve as mechanical cues for neurite regrowth. To promote vascular regeneration, therapeutic cells seeded in EngNT release pro-angiogenic factors that act as chemical cues for the formation of new micro-vessels [4]. A key question is then to find which therapeutic cell type, density and spatial distribution will lead to the best revascularisation and be able to sustain long term regeneration.

We address this challenge by combining experiments with simulations. We develop a system of continuous, coupled, non-linear, diffusion-reaction equations that we parameterize using a dedicated set of in-vitro experiments. Doing so allows us to describe the interplay between the therapeutic cells and their microenvironment, including cell proliferation, nutrient consumption, and growth factor secretion. We then overlay this continuous description with a discrete model for vessel dynamics that includes a description of vessel growth, blood flow and molecular exchanges between the vasculature and the surrounding tissue. Coupling these two models allows us to reproduce the rich spatio-temporal dynamics between blood flow, angiogenic processes, oxygen delivery, growth factors and seeded cell population during the early stages of nerve repair.

Simulations are performed for different therapeutic cell types and for a range of cell-seeding densities and spatial distributions to explore the impact on angiogenesis and cell survival. Results predict the spatio-temporal distribution of cell density, oxygen, and growth factor throughout the microvasculature and EngNT. In particular, they indicate that seeding cells beyond a given threshold appears to be detrimental for long-term cell survival and vascular regeneration but that seeding them preferentially close to the nerve stumps can help sustain gradient of growth factors in the nerve repair construct. This computational-experimental approach therefore allows us to explore efficiently a wide variety of scenarios and identify new cell seeding strategies that may accelerate revascularisation of a repair construct and improve cell survival to be taken forward to in vivo experimental testing.

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Novel Numerical and Analytical Techniques to Decouple Strain Energy Density in Materials with Poisson's Ratios Larger than 0.5

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Key Words: *Biomechanics and Mechanobiology, Constitutive Models, Collagen Constructs*

Introduction: Strain energy density (SED) is a scalar measure of deformation that can be decoupled into hydrostatic and deviatoric parts. Hydrostatic energy controls volume changes while deviatoric energy controls shape changes (distortion). Decoupling SED is a common practice in biomechanics as the different parts are predictive of biomaterial damage, growth, and remodeling [1]. Moreover, uncoupled SED formulations are often used by finite element (FE) solvers to avoid numerical issues when modeling nearly- and fully-incompressible material behavior [2]. However, a notable limitation of existing hydrostatic formulations used for decoupling is that they are only suitable for modeling materials with a Poisson's ratio close to 0.5; yet, many biomaterials, including ligament, tendon, and collagen gels, exhibit Poisson's ratios that greatly exceed 0.5. Therefore, continuum constitutive models used to describe soft tissue behavior generally do not reflect the volumetric material behavior seen experimentally. A need thus exists to develop a constitutive framework to decouple energy in materials with large Poisson's ratios. Here we present numerical and analytical methods for decoupling SED in materials with Poisson's ratios larger than 0.5.

Methods: The numerical approach consisted of decoupling stress and strain tensors in small increments of areas and numerically integrating the areas under the stress-strain pairs. A custom MATLAB function was developed to implement this technique and was validated using three test cases with known answers: uniaxial tension (T), uniaxial compression (C), and biaxial tension-compression (CT). For the analytical approach, we introduced a new mathematical expression for hydrostatic energy that was paired with a deviatoric Mooney-Rivlin counterpart. Cauchy stress was derived based on this new decoupled SED formulation and implemented in MATLAB. This code optimized model parameters to experimental data using the Levenberg-Marquardt algorithm. The numerical and analytical methods were used to decouple SED on type-I collagen constructs that displayed large Poisson's ratios over 0.5 and were subjected to different loads (T, C, and CT).

Results: The numerical approach accurately calculated total SED in all three cases with less than 0.02% error, and calculated deviatoric and hydrostatic SED with less than 0.4% error. The analytical approach proved successful in modelling both small and large Poisson's ratios (all NRMSE's less than 0.2%). Moreover, these approaches revealed that collagen constructs have a significant difference in hydrostatic and deviatoric energies due to loading condition, as well as a negative hydrostatic energy in the large Poisson's ratio cases (T, CT), which supports the observation that soft tissue can lose fluid under loading [3].

Conclusion: The numerical and analytical methods developed in this study will help investigate whether hydrostatic and deviatoric energy can predict damage, growth, and remodeling in native and surrogate soft tissue. Importantly, the analytical framework has the potential to be implemented in FE solvers, which would open doors for more accurate modeling of volumetric behavior in a plethora of materials that display large Poisson's ratios.

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A fluid-structure interaction model of brain tissue

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Key Words: *tissue stiffening, fluid-structure interaction, brain injury*

The biomechanical properties of brain play an important role in understanding the basics of brain injury and development [1]. While many constitutive representations of healthy brain tissue are emerging [2-4], studies have found brain tissue becomes less stiff following damage [5, 6]. Besides stiffness change, injured brain tissue had significant morphological changes of cerebral vasculature [5]. We hypothesize the structure formed by this vasculature plays a central role in the mechanical response of brain tissue both before and after injury, and may be a determinant of an individual's injury susceptibility. To investigate structural changes of brain tissue after injury, we constructed a fluid-structure interaction (FSI) model of brain parenchyma and studied how vessel size, cerebral spinal fluid (CSF) flow velocity, and CSF flow mode could change the biomechanical properties of brain tissue. A representative volume element (RVE) was constructed for compression and shear testing. Results showed the vessel size, flow velocity, and flow mode could affect the shear modulus of RVE during shear, but not Young's modulus in compression. These highlight the importance of considering cerebral vasculature as a structure in predicting and analyzing the brain's response to mechanical loadings before and after injury.

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An Electron Micrograph-Informed Axon Model Predicts Microstructural Failure Mechanisms

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Key Words: *Axon, Damage, Heterogeneity*

In the United States, over 1.7 million people sustain a traumatic brain injury each year, and about 5.3 million people are currently living with a traumatic brain injury-related disability [1]. While the trauma itself occurs at the larger spatial scale of the whole head, the damage can be traced down to the smaller scale of individual axons within the brain. Computational head trauma models predict axon injury by applying a damage threshold to the calculated strains. However, the current roadblock in accurate predictive injury simulation is the selection of the appropriate safety level threshold for axonal failure.

Previous studies have used computational models of the axon cytoskeleton to investigate how axons fail under applied loading [2]. These past studies have all assumed an idealized geometry with regularly spaced microtubules and constant cross-sectional areas; however, serial section electron micrographs show that microtubules vary in number and length along neurites [3]. Since the weakest cross section initiates failure in this heterogeneous cytoskeletal structure, simulations using an idealized geometry tend to overestimate axon strength.

To address this issue, we used electron micrographs to build an axon model with more realistic microtubule structure and compared its mechanical response to that of an idealized geometry. Using serial section transmission electron micrographs taken of a 15-um long section of a *C. elegans* touch receptor neuron [3], we established a semiautomated procedure to identify microtubules in these images and reconstructed the structure of the microtubule bundle within the neurite. We then discretized the microtubule geometry using beam elements in Abaqus Standard and added truss elements to represent crosslinking proteins. For comparison, we also created idealized models with constant cross-sectional areas equal to the smallest, largest, and average areas found in the electron micrographs. In the realistic geometry, simulations of tensile loading revealed localized regions of high strain corresponding to the weaker cross sections with fewer microtubules. On the other hand, the idealized models exhibited a more uniform strain distribution along the axon. Furthermore, for the same overall axon strain, the peak crosslink stretch in the realistic geometry exceeded that of the idealized geometries by a factor of 1.5. For a given total axon strain, the heterogeneous distribution of deformation along the realistic geometry results in a higher risk of failure compared to the idealized geometry. Our study shows that idealized geometries overestimate axonal strength and underestimate the risk of axonal damage. We anticipate that our new axon model more accurately represents the microstructural failure mode of the axon under mechanical loading.

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Mechanical stresses in brain folding inform spatial variations in cortical microstructure

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Key Words: *buckling, tissue remodelling, mechanical feedback, viscoelasticity, growth*

The mechanical and cellular processes that govern brain folding remain subjects of active research. Experimental data support a primary role of constrained cortical expansion, resulting in physical buckling, to drive the formation of gyri and sulci [1]. At the macroscopic level, computational models have provided useful exploration into the effects of mechanical feedback on developing brain morphology [2-3]. At the microscopic level, computational models require further development to understand the role of mechanical feedback on tissue-level changes.

Recently, we proposed a modelling framework in which biological behaviours, such as stress-dependent growth, may be assigned to specific cellular elements of brain tissue using volume fractions. By tracking changes in specific cellular constituents over time, this approach allows us to simulate tissue remodelling and infer microstructural changes that may result from mechanical factors. For example, by explicitly defining stress-dependent axon growth in terms of subcortical fiber volume fractions, models have predicted emergence of stereotyped anisotropy consistent with white matter organization [4]. In the present work, we extend this framework to consider microstructural remodelling in the cortex. We hypothesize that bending stresses resulting from cortical folding, such as increased compression in the superficial layers of sulci, contribute to differential patterns of cortical tissue anisotropy observed between gyri and sulci.

To probe cortical microstructure over the course of brain folding, we examined high resolution ex vivo diffusion tensor imaging from ferrets and rhesus macaques. We report stereotyped spatial patterns in diffusion anisotropy relative to gyri and sulci that are consistent with predictions of the computational model over the period of cortical folding. Thus, by simulating expected stress-dependent responses of specific tissue elements – including cell bodies, axons, dendrites, and extracellular matrix – in our model, we show that mechanical stresses resulting from folding may influence cortical microstructure in ways consistent with imaging and previously reported histological observations. As high-resolution diffusion tensor imaging becomes more common in research and clinical settings, these findings will provide context for the interpretation cortical FA maps as they relate to normal and abnormal brain development.

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Poro-Viscoelastic Effects During Biomechanical Testing of Human Brain Tissue

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Key Words: *Human Brain, Viscoelasticity, Poroelasticity, Constitutive Modeling*

In recent years, it has been recognized that mechanics play an important role for human brain development, injury and disease [1]. Due to its extreme complexity, different experimental studies characterizing the mechanical behavior of brain tissue have reported seemingly contradictory results concerning the stiffness difference between gray and white matter tissue [1]. Computational models based on the theory of nonlinear continuum mechanics have proven to be a valuable tool to understand the physical mechanisms underlying the tissue response and can assist a profound analysis of associated experimental data. While the observed discrepancies in experimental data can be attributed to different testing techniques varying in time and length scales, also different boundary and drainage conditions in combination with the biphasic, poro-viscoelastic nature of brain tissue affect the results [2, 3].

In order to investigate the influence of viscous and porous contributions to the tissue response under different loading conditions, we model brain tissue as a poro-viscoelastic material using a numerical framework based on the Theory of Porous Media [2]. We explore the effects of various material parameters on the numerical response for three experimental loading modes: large-strain cyclic compression-tension, stress relaxation in compression and small strain flat-punch indentation. Thereby, we observe a strong coupling between viscous and porous effects, highly depending on the yet unquantified intrinsic permeability. Our simulations can explain why indentation experiments indicate that white matter is stiffer than gray matter, while large-strain compression tests show the opposite trend, and reveal the utmost importance of appropriate experimental data analysis.

Through our systematic numerical simulations, we find that the extremely complex and nonlinear tissue behavior evoked by its biphasic nature, cannot be captured by a single effective modulus from indentation experiments at relatively low strains nor by maximum stresses during large-strain loading. Such values do not necessarily represent the actual stiffness of the material and might change depending on the loading and boundary conditions. Since the fluid flow within and across the boundaries of the sample is key to the overall tissue response, experimental setups should be carefully designed in the future to avoid unwanted effects and measure the particular property relevant for a certain application.

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Models and metamodels of spatially heterogeneous material domains

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Key Words: Machine Learning, Benchmark Datasets, Biomechanics, Spatial Heterogeneity

Using simulation to predict the mechanical behavior of heterogeneous materials has applications ranging from topology optimization to multi-scale structural analysis. However, full-fidelity simulation techniques such as Finite Element Analysis can be prohibitively computationally expensive when they are used to explore the massive input parameter space of heterogeneous materials. Therefore, there has been significant recent interest in machine learning-based models that, once trained, can predict mechanical behavior at a fraction of the computational cost. Over the past several years, research in this area has been focused mainly on predicting single Quantities of Interest (QoIs). However, there has recently been an increased interest in a more challenging problem: predicting full-field QoI (e.g., displacement/strain fields, damage fields) for mechanical problems. Due to the added complexity of full-field information, network architectures that perform well on single QoI problems may perform poorly in the full-field QoI problem setting. There are three components to the work presented in this talk. First, we introduce the Mechanical MNIST dataset designed to enable the investigation of full field QoI prediction. Second, we established strong baseline performance for predicting full-field QoI with MultiRes-WNet architecture. Third, we show results for creating generative models of spatially heterogeneous input patterns based on a limited number of examples to enhance a ML training dataset. In addition to presenting the results here, we have released our model implementations and datasets under open-source licenses. We anticipate that future researchers will directly use our model architecture on related datasets and potentially design models that exceed the baseline performance for predicting full-field QoI established in this paper.

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Biomechanics of Fetal Aortic Stenosis and Fetal Aortic Valvuloplasty

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Key Words: *Fetal Heart Biomechanics, Finite Element Modelling, Computational Fluid Dynamics, Fetal Heart Intervention, Congenital Heart Diseases, evolving HLHS*

Hypoplastic left heart syndrome (HLHS) is a severe congenital heart disease where the left heart and aorta are underdeveloped. Some HLHS developed due to fetal aortic stenosis and specific associated abnormalities during mid-gestation. Natural history of this condition showed that it led to progression to HLHS by birth in a majority of cases, thus the condition is known as evolving HLHS (eHLHS). In such patients, fetal aortic valvuloplasty could resolve abnormalities, induce better growth for some cardiac structures, and prevent progression to HLHS in some cases (66-72% biventricular births compared to natural history of 26-33%) [1,2]. Currently, little is known about the biomechanics consequences of the disease and intervention, although biomechanics stimuli are understood to guide cardiac development.

Here, we conduct image-based simulations to enable deeper understanding of eHLHS and intervention biomechanics, so as to inspire optimization of the intervention, and to enable better prediction of outcomes and more accurate patient selection, so as to improve efficacy. Both computational fluid dynamics (CFD) of blood flow mechanics, and finite element (FE) modelling of myocardial mechanics, based on 4D clinical echo images were conducted in conjunction with an age-scalable fetal Windkessel lumped parameter model.

CFD simulations demonstrated that eHLHS left ventricles (LVs) had a distinctively different flow dynamics, where mitral inflow occurred as a monophasic, narrowed and fast jet that transported a vortex ring directly to impinge on the apical region, leading to altered WSS spatial patterns. This was likely due to impaired mitral valve opening. Further, LV pressures, intraventricular pressure gradients, and energy losses were drastically higher than normal LVs. In post-interventional hearts, these abnormalities alleviated, but owing to aortic regurgitation from valvuloplasty injury, a narrow and fast aortic regurgitation jet that impinged onto the apical region dominated flow dynamics, retaining features of the altered WSS patterns.

FE simulations demonstrated that eHLHS hearts had drastically elevated LV and left atrial (LA) pressures and myocardial stresses and drastically reduced stroke volumes that depended on aortic stenosis severity, but these effects were moderated by mitral regurgitation. Myocardial hypertrophy often manifested that led to enhanced regurgitation severity, but contractility were likely reduced by cardiomyopathy. In the post-interventional LVs, de-pressurization of the LV could be attained to various extend, depending on extent that aortic stenosis was resolved. De-pressurization of the LA, however, depended further depended on the extent of aortic regurgitation, suggesting room for optimization on size of the valvuloplasty balloon. A workflow for quickly predicting acute outcomes from pre-interventional scan data was developed, which may improve on our currently poor ability to predict outcomes.

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Biomechanics of the Laminar Load-bearing and Neural Tissues with Body Position Change

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Key Words: *Body Position, Posture, Intraocular Pressure, Cerebrospinal Fluid Pressure, Optic Nerve Head, Finite Element, Ocular Biomechanics.*

The lamina cribrosa of the eye is continuously under intraocular pressure (IOP) and cerebrospinal fluid pressure (CSFP) from the anterior and posterior surfaces, respectively. A body position-dependent effect on the difference between IOP and CSFP may increase translaminar pressure (TLP), which that has been hypothesized as a possible risk factor in glaucoma pathogenesis. However, there have been few studies of the resultant stresses and strains within the lamina cribrosa trabeculae and interspersed neural tissues with TLP change. This study aimed to calculate the influence of postural change (sitting vs. supine) on the resultant stresses and strains in the optic nerve head, especially the lamina cribrosa beam and neural tissue, under simultaneously applied IOP and CSFP. Three eye-specific posterior microstructural finite element models were constructed, with circumferential, radial, and planar isotropic cable elements representing anisotropic collagen fibers embedded in the peripapillary sclera via a fully coupled, mesh-free, penalty-based beam-in-solid material-modeling algorithm. The FE models were then subjected to three different combinations of IOP and CSFP loading consistent with postural changes; results were then interpreted in relation to the postural role in the resultant optic nerve head deformations, stresses, and strains. The supine body position caused a larger tensile, compressive, and shear stresses and strains in the optic nerve head compared to the sitting position. IOP was the dominant (p<0.05) factor in the resultant stresses and strains in the laminar trabeculae and neural tissues compared to CSFP. IOP also was the dominant factor (p<0.05) driving deformations of the anterior and posterior scleral canal openings as well as anterior and posterior laminar insertions (~ 3 times larger than CSFP) while CSFP played a pivotal role in controlling the posterior laminar deformation. The cable elements representing the collagen fibers in the peripapillary sclera experienced a larger axial force in the supine compared to the sitting position, with IOP being the dominant factor compared to CSFP. Estimation of the resultant stresses and strains in the lamina cribrosa beams and neural tissues due to body posture could have practical implications for understanding the pathogenenic mechanisms of glaucoma and the ocular effects of idiopathic intracranial hypertension, as well as explaining visual impairment in astronauts in long-duration spaceflight.

From Patient-Specific Medical Images to Atrial Thrombosis Risk: Physics Informed Neural Networks and Multiphysics Simulations of Electrophysiology, Biomechanics, and Hemodynamics

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Key Words: *Atrial fibrillation, stroke, machine learning, fibrosis*

Cardioembolic strokes are a leading cause of mortality in atrial fibrillation (AF), the most common arrhythmia with an estimated lifetime risk > 33%. During AF, impaired atrial wall motion creates stagnant regions where clots can form, typically in the left atrial appendage (LAA). Current tools to predict stroke risk in AF patients are not personalized and have modest accuracy. This paper outlines image-based computational approaches aiming to improve our mechanistic understanding of LAA thrombosis and predict cardioembolic stroke risk. First, we consider multi-physics LA simulations resolving the electrophysiology (EP), biomechanics, and flow physics. The simulations are informed by patient-specific MRI data, including late gadolinium-enhanced scans mapping fibrotic regions. Of note, atrial fibrosis is clinically linked to stroke risk but the underlying mechanisms remain elusive. In our EP model, fibrotic areas have altered action potential dynamics (slowed upstroke and prolonged refractoriness) and impaired conduction. Besides, we model mechanical fibrosis effects by locally increasing stiffness and reducing peak contractile active tension. These models are coupled to a computational fluid dynamics (CFD) solver to calculate blood flow, hemostasis metrics (e.g., residence time), and the evolution of clot promoting chemical species (e.g., thrombin). Our simulations suggest fibrosis dramatically increases thrombogenic risk in patients with tortuously shaped LAAs. Second, we consider the problem of inferring LAA hemodynamics, hemostasis metrics, and the concentration of clot promoting species from the dynamics of a passive scalar (contrast agent) in 4D CT image sequences. We implemented reduced-order models (ROMs) based on simplified advection-diffusion equations for the contrast agent, residence time, and chemical species, as well as physics informed neural networks (PINNs) representing the whole flow physics. The ground truth was obtained from CFD simulations. We found that, while advection-diffusion ROMs fail to capture the fine-scale features of residence time and chemical species, they accurately infer their average values. Due to their low computational cost, ROMs are well suited for extensive parametric runs to derive optimal imaging settings and contrast injection profiles. On the other hand, when contrast injection is properly tuned, PINNs fully infer LAA hemodynamics using each patient's 4D contrast agent concentration fields from CFD as training data. Overall, these studies illustrate how computational modeling can interface with medical imaging at various points along the fidelity vs. translatability axis to shed light on the determinants of atrial thrombosis.

Generation of Dynamic High-Order Patient-Specific Biomedical Meshes from Medical Images Using an Advancing Front Approach

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Key Words: *High-order mesh generation, advancing front method, tetrahedral meshes, medical images, biomedical meshes, cardiac application*

Accurate biomedical simulations play an important role in aiding doctors with the diagnosis of and treatment of various diseases. High-order PDE solvers for biomedical simulations have recently attracted the interest of the computational science community since they yield accurate PDE solutions at a lower computational cost.

Most patient-specific geometric models and biomedical applications involve geometries containing curved surfaces. To represent the highly-curved geometries of the biomedical geometric models, high-order surface meshes with curved elements are used; these are paired with high-order volume meshes of the geometric domain's interior and high-order PDE solvers.

While various high-order mesh generation schemes have been developed, most of these methods require the geometric domain to be represented using a computer-aided design (CAD) model. However, CAD models are not readily available for biomedical applications. As such, the goal of our research is to develop a high-order mesh generation scheme that does not depend on use of a CAD geometry but instead generates high-order patient-specific meshes from medical images.

In this talk, we present our method for generating high-order patient-specific biomedical meshes from medical images [1]. To this end, low-order surface meshes are first obtained from the medical images. Next, these overrefined meshes are simplified and converted to high-order surface meshes. Our method then directly generates a high-order tetrahedral volume mesh using an advancing front approach. Finally, the mesh is smoothed to take advantage of the high-order degrees of freedom and to improve its quality.

We present several examples of high-order patient-specific biomedical meshes of soft tissues (e.g., liver and heart) and rigid tissues (e.g., bones) that our method generated from medical images. In addition, we present a dynamic cardiac application. For this application, the deep learning framework proposed in [2] was used to segment the cardiac chambers and estimate the cardiac motion from the cardiac cine magnetic resonance images.

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Imaging Informed Computational Models of Skin

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Key Words: *multiscale, multiphoton microscopy, microstructure, fiber networks, failure*

Skin is a complex, multilayered biomechanical structure, whose properties are dependent primarily on multiscale mechanical interactions that occur in the dermis. The dermis is a heterogeneous structure that largely consists of collagen, elastin, and proteoglycans. The composition and arrangement of these proteins, which can vary substantially with anatomic location, sex, ethnicity, age, and health, gives rise to its rich mechanical behavior. Although the biomechanics of skin has been studied for decades, new and interesting mechanical phenomena continue to emerge as new technologies become accessible. For example, the ability to observe both macroscale tissue deformation and microscale fiber-level restructuring has recently become possible[1]. These experiments use multiphoton microscopy during macroscale mechanical testing of mouse skin to acquire microscale quantitative data on collagen fiber density, organization, realignment, and kinematics. These experiments reveal that skin is not incompressible, that it exhibits large Poisson's ratios, and the fiber kinematics are non-affine with the macroscopic deformation of the tissue.

To better understand these data and their implications for explaining the mechanical behavior of skin, how the mechanical environment of skin changes with aging, and how aging leads to a higher susceptibility for tissue tearing, we have incorporated these data into a multiscale finite element model of the tissue. These imaging-informed mechanical models use volume averaging to connect a set of discrete microscale fiber networks to the macroscale mechanical behavior of the whole tissue. These models are able to capture many features of the complex behavior of the mouse skin observed experimentally. For example, the models were able to predict fiber restructuring within the sample gauge region, the force response, and the large decrease in volume observed with increasing stretch[2]. Models that were not informed with sample-specific details of the microstructure were not as accurate in their predictions.

We are now using these imaging-informed models to better understand the mechanism of tearing in skin as a function of age. To help localize the location of tissue failure for imaging purposes, dog bone shaped mouse skin samples were notched on one side of the center of the gauge region. The surrounding microstructure was imaged with multiphoton microscopy at each step of stretch. Models matching the sample geometry and boundary conditions were produced, and rules that break fibers that exceed a set stretch ratio were implemented. These models reveal an interesting pattern of restructuring around the notch that progresses laterally to the unnotched edge as the fibers fail. This behavior was also observed experimentally.

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Integrating Medical Imaging, Computer Vision, and Artificial Intelligence for Biomedical Modeling and Simulation Applications

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Key Words: *Medical Imaging, Artificial Intelligence, Computer Vision, Biomedical Applications*

Medical imaging has become an indispensable tool in medicine, enabling the diagnosis and treatment of previously debilitating diseases, by providing a patient-specific and patient-customized approach to therapy planning and guidance [1]. Medical imaging enables accurate and precise extraction of desired anatomical features, which, in turn, can be converted into virtual (and physical, thanks to 3D printing and rapid prototyping) replicas of the anatomy that can be used to model, simulate, plan and guide patient-customized therapies. Nevertheless, the pathway from medical imaging to biomedical modelling and simulation for biomedical applications entails the use of intelligent image computing and computer vision tools, many of which have been revolutionized by the latest development in artificial intelligence, which have been shows to achieve unmet performance, in terms of both accuracy, precision, and computational efficiency.

Our presentation as part of the *Imaging-informed Computational Modeling for Medicine* minisymposium will provide an overview of several tools and techniques that illustrate the power if integrating medical imaging, computer vision and artificial intelligence for several computational modelling and simulation applications in cardiology, image-guided robot-assisted interventions, and orthopaedic interventions. Specifically, we will present several deep-learning-based cardiac image segmentation and registration algorithms [2] that have enabled the creation of both static and dynamic surface and volume meshes of the heart [3] by capturing the geometry and deformation of cardiac features of interest from multi-dimensional medical imaging sequences, as well as their use for cardiac biomechanics simulations. Similarly, we will illustrate the performance of deep-learning-based image segmentation to automatically identify and label robotic instruments, in the effort to augment video sequences used for robot-assisted laparoscopic interventions [4]. Lastly, we will show how image-based characterization can be utilized to infer the biomechanical strength of bone to model and simulate optimal spine implant deployment.

In summary, this lecture will highlight several AI-enhanced computer vision tools that enable harvesting rich information from medical images to generate multi-dimensional 3D, 4D (3D + time) and 5D (4D + function) models of patient-specific anatomy or surgical instruments, to conduct simulations and provide new visualization to optimize computer-integrated diagnosis and therapy.

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Introducing an Inverse Finite Element Model of the Ventilated Lung

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Key Words: *Pulmonary Biomechanics, Inverse Finite Element Analysis, Digital Image Correlation, Lung Mechanics, COVID-19*

Despite millions of premature deaths and billions of dollars in medical costs annually, pulmonary research remains nascent and extraordinarily underdeveloped, continuing to undermine scientific breakthroughs as witnessed during the COVID-19 pandemic. Computer simulations are key to inaugurating novel lung therapies and medical devices, but often lack physiological relevance due to the absence of experimental data. Here we capitalize on the linkage derived from the local deformation behaviour of the inflating whole lung organ when subjected to global inflation pressures and volumes using our custom-designed electromechanical ventilator and digital image correlation (DIC) unique interface [1,2] in order to produce the first experimentally informed three-dimensional inverse finite element analysis (IFEA) computational model [3]. Multiple hyperelastic continuum formulations are utilized to determine the optimal set of material parameters using both derivative-based and gradient-free algorithms to minimize the error between simulation and experiment. This reduced-order, image-based, pulmonary surface model (representing the contributions of the bronchi, parenchyma tissue, and visceral pleura) captures the heterogenous and anisotropic characteristics of the distending lung. The resulting innovative pulmonary macromechanics framework can be used to explore various medical ventilation modes, predict regional pulmonary force and stretch distributions, and be further adapted to assess diseased lung mechanics.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Magnetic Resonance Imaging Informed Models of Cardiac Performance

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Key Words: Magnetic resonance imaging, Cardiac kinematics, Myofiber Strain, Cardiac modeling

Medical imaging provides a diversity of data for building patient-specific computational models of the heart. These models estimate performance variables that may not be measured directly (e.g., tissue stress and strain, hemodynamics, or electrical activity). Cardiac magnetic resonance imaging (MRI) can acquire time-resolved images that quantitatively encode myocardial displacements and microstructure. Herein, we summarize recent advances on how these data are acquired and fused using computational models to produce microstructurally anchored measures of patient-specific cardiac performance.

Cardiac MRI tagging and DENSE methods encode myocardial displacements in the magnitude and phase of the complex-valued MRI signal, respectively. The observed tagging motion or phase evolution can be decoded with conventional or machine-learning based image processing methods to produce a time-resolved material deformation mapping $\varphi(t)$ suitable for strain tensor ($\mathbf{E}$) calculations. $\mathbf{E}$ can be projected along a vector of interest ($\vec{v}$, e.g., circumferential or $\vec{c}$) to produce a specific strain component ($E_{vv} = \vec{v}\mathbf{E}\cdot\vec{v}$). Cardiac diffusion tensor imaging (cDTI) is an MRI technique that enables *in vivo* estimates of myocardial organization and produces a static pixel-wise estimate of the local diffusion tensor ($\mathbf{D}$). The primary eigenvector of $\mathbf{D}$ accords with the "myofiber" direction ($\vec{f}$). Hence, "myofiber" strain (E_{ff}) can be obtained using a suitable model that integrates $\mathbf{E}$ and $\mathbf{D}$. E_{ff} is microstructurally anchored and provides insight to cardiomyocyte performance, whereas E_{cc} is only a convenient geometric construct.

The most direct approach to estimate E_{ff} computes $\mathbf{E}$ by directly differentiating the deformation mapping measured with DENSE. Although efficient, differentiating the deformation mapping amplifies the experimental error. To overcome this problem, we estimate cardiac strains based on a kinematics model that contracts by imposing shortening along $\vec{f}$ measured from cDTI. By minimizing the difference between computed and measured motion, differentiating is avoided and subject-specific strains are then estimated.

The clinical adoption of these performance metrics requires validation of the methods used to compute them. Validation presents two challenges: 1) Evaluating image processing pipelines against a known ground truth; and 2) Measuring strain confidence intervals due to different processing pipelines and algorithms. In order to solve the first problem, we have developed a computational deforming heart model with known $\varphi(t)$. To solve the second challenge, we propose a cardiac kinematics benchmark problem to compare inter-method differences.

Ultimately, MRI informed models of cardiac performance may transform cardiac diagnosis by providing microstructurally anchored strains that can also be the input for simulations of cardiac mechanics, including the estimation of myocardial tissue properties and material law changes in disease.

Modeling Neuron Growth Using Isogeometric Collocation Based Phase Field Method

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Key Words: *Neuron Growth Modeling, Phase Field, B-splines, Isogeometric Collocation*

We present a new computational framework of neuron growth based on the phase field method and develop an open-source software package called "NeuronGrowth_IGAcollocation". Neurons consist of a cell body, dendrites, and axons. Axons and dendrites are long processes extending from the cell body and enabling information transfer to and from other neurons. There is a high variation in neuron morphology based on their location and function, thus increasing the complexity in mathematical modeling of neuron growth. We propose a novel phase field model with isogeometric collocation to simulate different stages of neuron growth by considering the effect of tubulin [1]. The stages modeled include lamellipodia formation, initial neurite outgrowth, axon differentiation, and dendrite formation considering the effect of intracellular transport of tubulin on neurite outgrowth. Through comparison with experimental observations, we can demonstrate qualitatively and quantitatively similar reproduction of neuron morphologies at different stages of growth and allow extension towards the formation of neurite networks.

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Numerical simulation tool for image-based bone healing process based on the Cartesian Grid Finite Element Method

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Key Words: Bone healing, Scaffold, Image-based simulation, Immersed Boundary Method.

Long bone fracture is usually stabilized with metal scaffolds like intramedullary implants. This technique implies two major surgeries, one for implanting the scaffold, and a second one for retiring the scaffold after the bone healing process has finished, which is mandatory according to practitioners and manufacturers due to possible long term negative effects [1].

We are involved in a project whose long term objective is to develop a numerical simulation tool for substituting the metallic implant by a bioabsorbable implant in order to avoid the second surgery. The first step of the process consist on simulating the bone healing process in order to obtain the daily mechanical requirements for the implant. Therefore, this work is focused on developing a numerical simulation tool for studding the patient-specific bone healing process. The technique used for that purpose is based on the Cartesian Grid Finite Element Method (cgFEM), successfully used in image-base simulation in the biomechanical context [2]. cgFEM allows to take into account the patient's bone medical image and bone remodelling process during the fracture healing process. In this case, the bone healing process is based on the use of fuzzy logic rules [3], showing a good correlation with experimental tests.

The numerical results provide information about the loads applied over the implant during the healing process, which is the starting point for the bioabsorbable implant design process.

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On the Sensitivity of Tricuspid Valve Models Built From Non-invasive Imaging Data

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Key Words: *Uncertainty, Clinical, Transcatheter, Repair, Predictive Modelling*

Clinically significant tricuspid regurgitation affects nearly 1.6 million Americans. Despite being termed a "public health crisis", few patients with functional tricuspid regurgitation (FTR) receive treatment. Moreover, 10-30% of patients that do receive treatment redevelop tricuspid regurgitation within a few years of surgery. We submit that these poor surgical outcomes are driven, in part, by an incomplete understanding of valve mechanics. Computer models built from patient-specific clinical data may be critical to this endeavour. However, building computer models from clinical data alone yields many challenges. Specifically, clinical imaging modalities such as ultrasound are unable to faithfully capture the intricate network of chordae tendineae that tether the valve leaflets. Additionally, tissue stiffnesses estimated through imaging-based inverse analyses are often orders of magnitude larger than those measured *in vitro*. Thus, we are faced with uncertainties in valve geometry and tissue material properties that limit our ability to accurately model the tricuspid valve. In this work, we examine the sensitivity of finite element models of the tricuspid valve to such uncertainties. To this end, we first obtain human tricuspid valves with FTR from hearts explanted after transplant surgery. Before the hearts are explanted, we record ultrasound images of the tricuspid valve in addition to valve hemodynamics. We then create an imaging-based finite element model of the regurgitant valve in absentia of any high-fidelity patient-specific data. Specifically, in this model we use an ultrasound-derived valve geometry, vary material properties based on values provided in existing literature, and use a topology optimization scheme to vary chordal configurations [1]. Through finite element simulations of the valve at end-systole, performed in Abaqus/Explicit, we determine the sensitivity of the imaging-based valve model to varied material properties and chordal configurations. Furthermore, to validate this model we use our previously established modelling framework to characterize the explanted tissue and build a high-fidelity finite element model of the same regurgitant tricuspid valve [2]. We then quantify the difference in predicted stresses between the high-fidelity and imaging-based valve models. Quantifying and analysing model sensitivities is essential to the advance of predictive modelling in biomedicine. In the future, predictive tricuspid valve models may be used for pre-surgical planning and medical device optimization which may help improve tricuspid valve repair outcomes.

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Quantitative Stretch-Induced Collagen Fiber Recruitment and Microarchitecture Changes Using Instant Polarized Light Microscopy

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Key Words: *polarized light microscopy, collagen, crimp, deformation, biomechanics*

Collagen architecture plays a central role in the biomechanics of soft tissues. While much has been learned about the macro and meso-scale mechanical properties of collagen, far less is known about the microstructural basis for tissue behavior, especially in tissues with complex microarchitecture. Polarized light microscopy (PLM) is a label-free imaging technique that has been widely used to visualize and characterize collagen architecture. However, quantitative PLM requires acquiring and analyzing multiple images, which complicates time-sensitive mechanical testing and microstructural analysis. We recently presented instant polarized light microscopy (IPOL) that allows label-free and direct visualization of collagen microstructure and orientation. IPOL leverages the full spatial resolution of the microscope-camera system, and its acquisition rate is only limited by camera speed. We demonstrate the IPOL-based tool by analyzing stretch-induced recruitment and deformation of tissues from the highly complex optic nerve head region.

Samples from the posterior pole of a sheep eye were prepared using sectioning techniques. The samples were then mounted on a custom micro-stretcher system and the stretching process was imaged with IPOL. Here we highlight three observations: First, the crimped collagen fibers in the peripapillary sclera (PPS) and lamina cribrosa (LC) beams straightened under stretch. At the initial state, the waviness (standard deviation of orientation) of crimp was significantly higher in the PPS (10.3°±2.6°) than in the LC (8.3°±2.5°). In addition, the uncrimping rate in the PPS (0.9±0.5) was significantly steeper than that in the LC (0.6±0.3°). This indicates PPS stiffening at a lower level of stretch, which could help protect the neural tissues in the LC from excessive mechanical insult. Second, we observed that stretch-induced PPS deformation was non-affine and inhomogeneous. Local deformations at the micro-scale varied greatly, even between adjacent collagen bundles. This indicates that resident cells may bear substantially different mechanical input even if only a few micrometers away. Third, at the micro-scale, the tissues do not behave in good accordance with some of the common assumptions of continuum mechanics. For instance, the tissues do not show conservation of volume or stretch-induced necking. Thus, to understand tissue and cell behavior it is necessary to develop more advanced models.

In conclusion, IPOL allows visualizing and quantifying collagen microarchitecture changes with stretch. This technique provides data that helps understand how the complex nonlinear properties of tissues arise from the collagen fiber microarchitecture. The experimental measures of collagen microarchitecture changes help drive fiber-based constitutive model formulations.

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Regional Variation of Corneal Stiffness with Keratoconus Progression

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Key Words: *Corneal stiffness; Keratoconus*

Purpose: To evaluate the regional corneal biomechanical deterioration with keratoconus (KC) progression as measured by the stress-strain maps (SSI)

Methods: In this retrospective record review, the preoperative of progressive KC cases that were submitted to corneal cross-linking (CXL) were evaluated. All cases were examined with Pentacam HR and the Corvis ST (Oculus, Wetzlar, Germany). Significant progression was based on the Pentacam's ABCD system. The SSI Maps were built on the first and last visits using numerical modelling based on the finite element method [1,2]. Through inverse analysis of patient-specific corneas the regional variation of mechanical stiffness across the corneal surface was determined.

Results: A total of 29 eyes were included. The cases presented the disease in different stages with maximum anterior curvature (Kmax) of 54.37 ± 4.55 D (44.5 – 64.4) and minimum thickness of 468.55 ± 27.74 μm (414 – 520). The mean age at the last exam before the CXL procedure was 20.1 ± 7.0 years (9 – 40). The mean time between the two examinations was 17.1 ± 17.1 months (1.4 – 58.4). The bIOP showed minimum non-significant alteration between the two exams (-0.08 ± 1.21 mmHg, range: -2.0 to 2.3, $p = 0.584$). The overall corneal stiffness as measured by SSI value in 8mm diameter presented slight but significant reduction from the first to the last exam (-0.02 ± 0.02, range: -0.09 to 0, $p < 0.001$). The regional reduction in stiffness was concentred in the area inside the cone. The SSI values inside the cone were significant lower in the last exam (-0.15 ± 0.09, range: -0.42 to -0.01, $p < 0.001$), while the SSI outside the cone presented minimum non-significant difference (0 ± 0.01, range: -0.04 to 0.01, $p = 0.999$).

Conclusions: It has been observed through the SSI maps that the regional deterioration in stiffness was concerted inside the cone area, while only mild non-significant alteration was observed outside the diseased area.

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Revealing Swallowing Mechanics by using Muscle-driven Computer Simulation Created based on Four-dimensional Computed Tomography and Muscle Anatomy

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Key Words: *Swallowing Simulation, Four-dimensional CT, Muscle Anatomy, Muscle Activity*

The swallowing mechanics is still unclear. The swallowing is an intrinsic motion consisted of both transporting food bolus from the mouth to the esophagus and preventing from entering the trachea. Although the functional anatomy supposes 38 kinds of muscles activating the tissues, the mechanics between the tissue motion and the muscle activity and the food bolus flow has been not revealed. One of the breakthrough methods to reveal the mechanics is a computer simulation based on the medical images and the anatomical knowledge.
A computer simulation for swallowing needs both a tissue model and a food model. The tissue model consists of rigid models like the hyoid bone and elastic models like the tongue. The tissue model needed three steps to be created. The first step was to segment the tissues on images obtained from the four-dimensional Computed Tomography (4DCT) for swallowing. The second step was to adjust the muscles to the tissues. The third was to arrange particles to the muscles. The particles were calculation points for the simulation. The food model was created using its physical properties. The simulation method was a coupled analysis using the moving particle method which was one of the meshless methods. The muscle activity was obtained from the linear search method of the optimization calculation.
The result indicated that the muscle-driven swallowing simulation clarified all the tissue motions including the wave movement of the tongue, the pharyngeal constriction and elevation, the arytenoid movement and the opening of the upper esophagus. Moreover, the tissue motion changed the way as the muscle activity increased or decreased.
The muscle-driven swallowing simulation provided the precise soft tissue motion as well as the muscle activity which were unable for the 4DCT. The imaging-informed computer simulation will be able to reveal the whole mechanics on eating including mastication and swallowing.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Understanding and predicting arterial elasticity by deep learning

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Key Words: soft tissue, constitutive modeling, machine learning

Constitutive modeling of soft biological tissues has rapidly gained attention over the last 20 years. The microstructure and macroscopic mechanical properties of soft tissues like arteries are closely related. Histological anylsis, modern imaging, and biomechanical testing have deepend our understanding of these complex interrelations. However, predicting the mechanical properties from microstructural information yet remains an elusive goal.

To address this problem, we introduce a novel machine learning framework that combines advanced theoretical concepts with deep learning [1]. Using data from mechanical tests, histological analyses and advanced imaging, this architecture is trained to predict the nonlinear macroscopic mechanical properties of arterial tissue. The incorporation of substantial prior knowledge from continuum mechanics and materials theory enables our architecture to learn already from small amounts of data ($10^1 - 10^2$ samples) to predict the stress-strain curves of soft tissue with high accuracy ($R^2 > 0.9$). To the authors' best knowledge, this is the first time that macroscopic mechanical properties of soft tissue are predicted with such high accuracy from the tissue microstructure. Moreover, we demonstrate that our machine learning architecture is not limited to predictions but can also help to understand the mechanics of soft tissue. Using advanced concepts of explainable artificial intelligence, we demonstrate that it enables the automatic, systematic and largely unbiased quantification of the importance of different microstructural features for the macroscopic mechanical properties.

The machine learning framework we present bears promise to be transformative for our understanding of soft tissue mechanics and to provide new insights into the changes of soft tissues during aging and various diseases.

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Using Digital Image Correlation to Validate a Finite Element Damage Model of Human Meniscus

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Key Words: *Soft Tissue, Continuum Damage Mechanics, Image-Based Model Validation*

Introduction. Meniscus tears are one of the most common orthopaedic injuries,[1] and surgeries to repair these tears are unable to effectively restore the native meniscus function. In order to help prevent meniscus tear injuries and improve surgical treatments, continuum damage mechanics (CDM) finite element (FE) models can be used to better understand the failure mechanisms and predict the loading conditions that cause tears to develop. However, the validation of these model formulations require comparisons to experimental data.[2] Digital image correlation (DIC) paired with high-speed video can be used to track tissue strains up to the moment of tissue rupture, enabling a precise comparison between model and experimental strains in the failure region.

Methods. Symmetric 1/8th dumbbell shaped coupons were built and analysed using FEBio studio (16144 elements).[3] Model parameters were tuned to stress-strain data from 10 monotonic tensile tests of human meniscus[4] using a transversely isotropic constitutive model. Damage evolution was modelled using a quintic polynomial with either von Mises stress criteria along the circumferential fibers, or 1st principle Lagrange strain criteria normal to them. The Lagrange strains and orientation of the tear region predicted by the model were compared to results from the DIC experiment.

Results. The selected model formulation provided average R^2 fits of 0.99 ± 0.01 for experimental data tested along the circumferential fiber network, and 0.97 ± 0.03 for data normal to the fibers. The concentration of maximum damage closely resembled the orientation of tissue ruptures from experimental data, with an oblique angle when loaded along the fiber axis, and a perpendicular one when loaded transversely. The model strains measured in this failure region were on average one-half to one-third those measured experimentally.

Conclusion. The excellent fits to experimental data, as well as the agreement between model and experiment regarding the tear orientation, suggest the selected constitutive model is appropriate to capture the anisotropic tensile failure behaviour of human meniscus. However, the inability of the FE model to correctly predict the high concentration of surface strain in the tear region indicates a potential limitation of CDM for modelling soft tissue failure. This study is the first to use full-field strain data to validate a damage model of meniscus tissue, and the results serve as an important advancement of failure theory for soft tissue and computational modelling of knee injury.

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A viscoelastic modelling of bone with microstructures

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Key Words: Bone, Mircostructure, Brick-and-Mortar, Viscoelasticity

Many biological materials behave attractive properties and attract scientists to investigate ingredient and architecture of the materials. Among the natural materials, bone can be recognized as a biocomposite, which consists of mineral and protein, and features higher toughness than its individual ingredient. This characteristic gives a impetus to explore the bone further. The well-know theory for the mechanical behavior of bone with consideration of its microstructure, which is usually called ”brick-and-mortar“, is the tension-shear chain model [1] which can well capture the elastic modulus of bone [2]. The present study proposes a viscoelastic model of bone taking into account the brick-and-mortar microstructure and addresses the exact solutions of the viscoelastic model under stepwise, constant-rate, and cyclic loading paths. The comparison between the response of the viscoelastic model and experimental data of bone under monotonic loading shows an accepted result. The influence of mircostructure on the mechanical properties of the bone including the creep function, the relaxation function, the instantaneous modulus, the asymptotic modulus, the complex modulus, the storage modulus, the loss modulus as well as the loss tangent are investigated.

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An elastoplastic model of cortical bone and its return-free integration

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Key Words: Cortical Bone, Elastic-Plastic Material, Anisotropic Material, Tension Compression Asymmetry, Numerical Integration, Return-free integration.

Bone with the volume fraction of mineral more than 70 % is usually classified as the cortical bone (or so-called compact bone). The mechanical features of the cortical bone including the anisotropic and the pressure-sensitive response as wall as the yielding asymmetry in tension and compression and slight hardening have be widely observed. In the present study, we propose an elastoplastic material with an anisotropic elastic part, an associated flow rule with anisotropic-pressure-sensitive yield surface, a nonlinear isotropic hardening, and a nonlinear kinematic hardening to model the mechanical behavior of the cortical bone. In order to calculate the accurate simulation of the model, we consider the strain control cases as wall as the mixed control cases and develop the return-free integration of the model which is underpinned the internal symmetry of the Lie group $\mathrm{SO}(n,m,\mathbf{g})$ transformation, where the metric $\mathbf{g}$ is singular, and automatically updates the stress on the yield surface during plastic phase. The capability of the return-free integration is tested by the error analysis including consistency errors, average errors, and iso-errors. It shows the return-free integration of the model for the cortical bone is stable, acceptable, and reliable. Further, accurate simulation of the cortical bone based on the return-free integration enable us to investigate the mechanical behavior of the bone under different loading conditions.

Computational Insights into the Conformational Changes of Matrix Metalloproteinase in the presence of Nanoplastics

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Key Words: *Extracellular Matrix, Nanoplastics, Molecular Dynamics Simulations*

Extracellular matrix degradation is a necessary process for numerous physiological and pathological events such as morphogenesis and wound healing, and matrix metalloproteinase-8 (MMP-8) is the major peptidase in the extracellular matrix that can catalyze several molecules, including aggrecan, gelatin, and collagen types I, II, III, VII, VIII, and X. The pollution of nanoplastics is of growing concern owing to their potential negative impacts on organisms. Nanoplastics are plastic particles with diameters less than 100 nm. Since nanoplastics are at least two orders smaller than eukaryotic cells, they are possible to penetrate into cells and influence organisms in molecular level. Moreover, nanoplastics have been found in the circulatory system of organisms. However, it is still unclear that how nanoplastics impact biological tissues after entering our body. Here we introduce a molecular dynamics approach to gain an insight into the effects of different nanoplastics on extracellular matrix degradation. It is found that different kinds of nanoplastics can cause different degrees of enzyme conformational changes, and they all influence the catalytic function of MMP-8 in different aspects. Our study shows the effects of nanoplastics on functional protein from an atomic-scale perspective, illuminating the urgent need for further understanding about the effects of various nanoplastics on other biological materials.

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Molecular Dynamics Study on Mechanical Properties of Polyethylene Glycol / 2-Hydroxyethyl Methacrylate Organogel with Lithium Chloride

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Key Words: *Organogel, Molecular Dynamics, Soft matters, Mechanical Properties*

Organogel[1] is a class of gel composed of organic solvent and cross-linking polymer network structure. The network structure within this material not only fixes organic solvent but also provides excellent mechanical stretching properties[1]. However, conventional organogel is unable to withstand high tensile stress. Recently, it has been found that by adding metal ions[2], the organogel can reach high failure stress and remain its high stretching property at the same time. While knowing that metal ion may increase crosslink density, the thorough mechanism is still unclear[2]. In our study, we focus on adding lithium chloride (LiCl) in polyethylene glycol (10-mer PEG) / 2-hydroxyethyl methacrylate (100-mer HEMA) organogel to study the strengthen mechanism.

Molecular dynamic simulation is used to study the difference between organogel and ionized organogel. We create two molecular models: pure PHEMA-PEG organogel and LiCl PHEMA-PEG organogel, and perform equilibrium simulation under NPT-ensemble with 300K and 1 atm. End-to-end distance, radius of gyration and persistence length of PHEMA and PEG are measured to understand the changes of polymers structure in two systems. Numbers of hydrogen bond and lithium-oxygen coordinate bond are analyzed. Finally, we perform tensile stress to study the modulus and structural change of the systems at the micro scale.

In LiCl PHEMA-PEG organogel system, we observe that end-to-end distance, radius of gyration and persistence length of PEG polymers decrease due to the effect of lithium ions. The number of hydrogen bond decreases from 974.69±71.35 to 770.61±38.62 while the number of lithium-oxygen coordinate bond between lithium and polymers dramatically increases, implying that the LiCl system has higher capability to withstand higher tensile stress. A higher density of crosslink of LiCl system implies that LiCl system is more stable and connected due to the coordinate bonds. Finally, from the tensile stress simulation, we obtain higher young modulus in LiCl than in pure PEG-PHEMA organogel.

In this research, we use molecular dynamic simulation to study the structural and mechanics difference of organogel and ionized organogel, and provide the explanation of the mechanism of the better mechanical behavior of the ionized organogel. From our result, it is shown that although lithium competes the oxygen in hydrogen bond, leading to a decrease in hydrogen bonds, the substituted lithium-oxygen coordinate bonds not only increase the stability, but also increase the failure stress of LiCl system. The findings from the atomistic modeling may help engineers to develop various functional organogel.

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Yield surface evolution of trabecular bone

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Key Words: Trabecular bone, Voronoi Honeycombs, Yield surface Evolution, Finite Element Method

The present study investigates the yield surface evolution of trabecular bone in an axial-shear stress space via the finite element analysis. A representative element or so-called unit cell of the trabecular bone is constructed with the microstructure of voronoi honeycombs and the initial and subsequenct yield surfaces of the representative element are probed. To model the mechanical property of trabecular bone, the relative density of voronoi honeycomb is 40 % and a bilinear elastoplastic material with asymmetric yield point in tension and compression is modelled in the finite element analysis. According to determination of yield point in the classical experiment of metal, the finite element analysis is conducted to simulate the uniaxial test and show the equivalent plastic strain of the voronoi honeycomb, then the proper determination of yield point in finite element simulations for the voronoi honeycombs is selected. The present study further extends the selected definition of yield point for 1D stress space to detect yield surfaces of the honeycomb in the axial-shear stress space via radial probing paths. Besides the initial yield surface of trabecular bone is detected, the bilinear pre-loading paths of displacement are applied to the voronoi honeycomb and the subsequent yield surfaces of trabecular bone are obtained. The observation on the finite element simulations shows the shape and the area of yield surface vary in different pre-loading paths of displacement.

Compressive Instabilities cause Densification Patterns in the Fibrous Extracellular Matrix, Facilitating Cell Migration and Invasion: Discrete Model Predictions

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Key Words: *ECM Mechanics, Compression softening, Fiber compression instability, Fiber alignment, Intercellular communication*

Biological cells embedded in fibrous matrices actively remodel the surrounding network by inducing unique deformation patterns. These patterns include tracts of elevated densification and fiber alignment and have been shown to regulate significant cellular processes such us cell migration and invasion [1] and intercellular communication [2]. Understanding the mechanism underlying these phenomena is equivalent to characterising the mechanical properties of Extracellular Matrix (ECM) fibers.

Previous studies on fiber mechanics revealed unusual mechanical effects partly dictated by their hierarchical structure. These effects include multiple regimes of stress-strain responses under compression marked by transitions from hardening to softening [3,4]. Based on this evidence and moving beyond a previous continuum instability model [5] to include the crucial effects of discreteness, here we develop a discrete fiber network and implement various constitutive relations to explore fiber mechanical behavior under cell-induced loading. Our simulations reveal two distinct mechanisms of fiber and fiber group compressive instability due to buckling and identify matrix densification in the form of tethers connecting neighbouring cells and radial bands emanating around each cell, as a direct effect of these instabilities. Statistical inspection show enhanced alignment of tensed fibers along the direction of the densified zones while severely compressed fibres locate in the transverse direction, as experimentally observed. We show that both fiber alignment and matrix densification are prevented in the absence of elevated compression. Our models demonstrate that compression instability is a key player for both ample fiber alignment and matrix densification, rendering compression softening as the dominant nonlinear mechanism in fibrous ECM. This sets new insights in exploring fiber response to cell-induced deformations and its implications to intercellular biomechanical interaction.

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Angioscopy Visibilities for Stenotic Arteries using Computational Fluid Dynamics

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Key Words: *Angioscopy, Flush, Computational Fluid Dynamics (CFD), Step injection, stenosis*

An angioscopy is an intravascular endoscopy device to visualize the colored interior of the blood vessel by delivering the endoscope to the arterial lesion using a catheter. Since the presence of blood flow usually blocks the view of the endoscopic camera, a transparent fluid flow, known as the flush flow, is needed to create a clear field of view between the camera and the arterial lesion, in order to obtain better quality images. In a previous study, we reported that using a step injection method, the visible area ratio of wall was 17-folds as large as that of using the conventional constant injection method; moreover, the optimised design of catheter also improved the visible area [1]. However, only a straight blood vessel was examined in the previous study, while the flushing behavior and effect of the step injection method on blood vessel in other geometries with more realistic feature remains unknown, which can be interesting and useful. Therefore, this study aims to evaluate the visibility of arterial walls in stenotic blood vessels using the step injection method.

Three stenotic models of coronary vascular wall were constructed using CAD software. The stenosis models represented a ball-shape, bilateral-shape, dome-shape, respectively. A step injection (180 mL/min *0.5 pulse) and the conventional injection (90 mL/min) flush was respectively applied to the inlet. ANSYS CFX 2020 R1 was adopted as a solver for the transient fluid flow simulation (1 pulse=1 sec). Then an integral of visible area ratio in a pulse (ARvar) was calculated for quantitative comparisons to the conventional injection.

Sections of the wall and the stenosis were observed from the camera viewpoint. The step injection created 1.4~7.0-folds higher ARvar than the conventional injection method in all models with different stenotic shapes. Especially, the bilateral-shape showed the highest ARvar, on the other hand, the ball-shape had the lowest ARvar. Compared to the straight artery, the effect of step injection is still higher than the conventional injection. However, the increase of visibility by step injection is smaller, especially the ball-shape.

In conclusion, the step injection to stenotic artery shows higher visibility of arterial wall compared to the conventional constant injection.

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Endovascular Simulation System to Improve Mechanical Thrombectomy for Acute Ischemic Stroke

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Key Words: *Mechanical Thrombectomy, Acute Ischemic Stroke, Vessel Tortuosity, Clot Stiffness*

Introduction: Mechanical thrombectomy with a stent retriever and/or aspiration catheter has been established as gold standard treatment for large vessel occlusion (LVO) in acute ischemic stroke (AIS). The first-pass effect, defined as successful complete or near-complete recanalization in the first attempt, has been associated with better clinical outcomes. Although high recanalization rates are reported with the advancement of devices and techniques, the rate of the first-pass effect is still approximately thirty percent. Therefore, it is imperative to understand the mechanisms underlying thrombectomy failure for early recanalization of LVO.

Several challenges in mechanical thrombectomy have been reported, such as tortuous anatomy of the vessels and stiff clots. However, the mechanisms for poor results in case of these challenges remained unknown. The aim of this study is to assess a new-generation aspiration system with hydro-separator technology that works regardless of clot size or composition.

The aim of this study is to examine the impact of vessel characteristics and clot stiffness on the performance of thrombectomy devices or techniques and to improve the efficacy and safety of stroke therapy.

Methods: We created artificial clot analogues with diverse stiffnesses and intracranial vascular silicone models with several tortuosities. The success rates of thrombectomy and vessel retraction force were evaluated in standard and challenging situations in realistic vascular models.

Results: Both the severity of vessel tortuosity and clot stiffness significantly affected the success rates of recanalization in simulated models. We observed that stent retrievers were stretched, collapsed in curved vessels, and lost clots in curved vessels. In addition, aspiration catheters ingested soft clots but not moderately stiff clots, whereas fragmentation of soft clots were observed with stent retrievers, although relatively stiff clots were well-integrated and removed. Aspiration catheters and stent retrievers with newer technology lead to significantly higher success rates than conventional devices.

Conclusions: Challenging situations were successfully created in 3D intracranial vessel models. This thrombectomy simulation system was useful to understand the underlying mechanisms of difficulties and to improve clinical decision-making in challenging situations.

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Generation of Virtual Patient Cerebral Arteries Focused on Geometric Feature Distributions Using Multivariate Normal Distribution

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Key Words: Virtual Patient Data, Cerebrovascular, Geometric Feature, *Multivariate Normal Distribution*

In recent years, methods to generate virtual patient database of artery geometry have attracted much attention due to the lack of sufficient database of medical images. B. Thamsen et al. generated a database of vascular geometries by the Statistical Shape Model (PCA-SSM) using Principal Component Analysis [1]. However, the basic concept of PCA-SSM does not contain the correlation of landmark points position [2]. Then, landmark points without the correlation can generate the unrealistic geometry on anatomical aspect. Recently, a method for generating virtual patient database assuming a multivariate normal distribution (MVND) method are proposed based on covariates such as age, weight, gender, and blood pressure [3]. This MVND method enables to generate a large set of variables with correlation. In this study, we introduce the method on generating a virtual cerebral artery database using the MVND method. The generated database was evaluated by the distributions of geometric features of the generated shape database.

The position of the 3D vascular centerline was extracted from MRA data. The centerline was divided evenly for each artery part: basilar artery (BA), left and right internal carotid arteries (ICA). We examined the number of equipartition 2 to 30 for BA and 2 to 100 for ICA. We assumed that the coordinates of x, y, and z at the equipartition points and the corresponding inner diameters d follows MVND. According to MVND, point groups and corresponding inner diameters were generated for 100 patients at each artery part. B-spline interpolation was performed with point groups to create a virtual patient database. The distributions of geometric features of the virtual patient database were compared with that of real patient database using length, tortuosity, curvature, and SOAM (sum of angle metric).

For BA and ICA, the distributions of length, tortuosity, and curvature of the virtual patient database were generally similar to those of the real patient database. However, in case three equipartition points were selected, the BA curvature distribution of the virtual patient database did not fit that of the real patient database. Therefore, virtual patient database using MVND may represent the real database with the complexity of cerebral arteries' bent if enough equipartition points number and B-spline interpolation are selected.

Virtual patient database of BA and ICA were generated using the MVND method. The distributions of the geometric features such as length, tortuosity, and curvature were similar to those of the real patient database, which suggests that this method is effective.

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Ionic mechanisms of ST segment elevation in electrocardiogram during acute myocardial infarction

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Key Words: *Myocardial infarction, ST elevation, Simulation, Solid angle*

Computer simulation provides a unique opportunity to examine the relationship between microscopic findings and clinical observations. We previously developed a multi-scale model of the human heart and torso, which can reproduce the surface ECG based on the ionic currents of cell models of electrophysiology(1) (2) (3). In this study, we applied this heart model to examine the ionic mechanism of ST elevation on an electrocardiogram that is a hallmark of acute transmural ischemia. However, the underlying mechanism remains unclear. We hypothesized that high ischemic sensitivities of epicardial adenosine triphosphate(ATP)-sensitive potassium (IK_{ATP}) and sodium (INa) currents play key roles in the genesis of ST elevation. Using a multi-scale heart simulation under moderately ischemic conditions, transmural heterogeneities of IK_{ATP} and INa created a transmural gradient, opposite to that observed in subendocardial injury, leading to ST elevation. These heterogeneities also contributed to the genesis of hyper-acute T waves under mildly ischemic conditions. By contrast, under severely ischemic conditions, although action potentials were suppressed transmurally, the potential gradient at the boundary between the ischemic and normal regions caused ST elevation without a contribution from transmural heterogeneity. Arrhythmias were observed under hyperkalemia with preserved ATP concentration. Slow conduction in the ischemic region may play a key role in the development of arrhythmias. These results provide the comprehensive understanding of the ionic mechanisms of ECG changes during transmural ischemia.

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Numerical simulation of the evolution of an intracranial aneurysm with pathological tissue remodeling

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Key Words: *hemodynamic factors, wall shear stress, aneurysm*

An intracranial aneurysm (IA) is local ballooning of a cerebral artery. Historically, various hemodynamics indices have been proposed as etiologic factors of the development of intracranial aneurysms. However, which factor(s) is true remains controvertial. To sort out hemodynamic indices and shed light on the etiology of the disease, we are developing a numerical framework of the aneurysmal development, which accounted for an interactive linkage between hemodynamics, vascular wall mechanics and biological responses.

The aneurysmal evolution was simulated by cyclically repeating three steps; blood flow simulations, tissue remodelling and deformation. Given vascular geometry, blood flow was simulated to obtain hemodynamic indexes such as wall shear stress (WSS), and oscillatory shear index (OSI). The amount of vascular components such as elastin and collagen were then locally changed based on the magnitude of the hemodynamic indexes to mimic pathological tissue remodelling. Finally, the vascular geometry was updated by defomration analysis with internal pressureliziation at a physiological pressure. Cyclically repeatitive implementation of these steps provided the aneurysmal evolution associated with pathological tissue remodelling.

We illustrate its application to rat experiments where de novo aneurysms formed at the bifurcations created by end-to-side anastomoses with the bilateral common carotid arteries [1]. Blood flow simulations demonstrated high WSS, high WSS gradient (WSSG) at the apex of the anastomosis for flow impingement, and high OSI at the entire region of the anastomosis for recirculation. When high WSS and high WSSG were used combinedly as the driving factor, the aneurysm evolved at the apex. When OSI was adopted, the blood vessel bulged entirely near the anastomosis. The aneursms formed looked similar to the correponding rat experiments. These results suggest that a combination of high WSS and high WSSG, and high OSI are possible candidates of the driving factors of the aneurysm evolution.

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Patient-Specific Biomechanics of the Right-Noncoronary Bicuspid Aortic Valve and Age-Matched Tricuspid Aortic Valve Control

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Key Words: *fluid structure interaction, hemodynamics, biomechanics, computational modelling*

Objective: Bicuspid aortic valve (BAV) is the most common congenital cardiovascular defect (1-2% of all live births) characterized by the abnormal formation of two rather than three cusps. Approximately 50% of young adults with BAV, mostly fusion of the right and noncoronary (R/NC) cusps, develop premature calcification leading to aortic stenosis by age 35.[1] The etiology of premature calcification in BAV is poorly understood, but mechanical contributions are implicated. Computational studies of the mechanical stimuli along BAV cusps have focused on adult cohorts after onset of calcification. Our objective was to create fluid-structure interaction (FSI) simulations of young BAV patients to elucidate BAV-induced mechanical stimuli prior to calcification.

Methods: Magnetic resonance imaging of 23 y/o patients with R/NC BAV (n=1) and a healthy tri-cuspid aortic valve (TAV, n=1) were conducted after IRB approval. Aortic and coronary artery morphology were extracted using SimVascular (simvascular.github.io). Valve cusps were constructed in SolidWorks (Dassault Systems) using dimensions made patient-specific by scaling to sinus geometry.[2] Physiologic boundary conditions (BCs) were implemented including measured pressure at the aortic inlet, a lumped-parameter model of downstream physiology at the aortic outlet, and flow imposed at coronary artery outlets. Hyperelastic anisotropic material properties were applied using biaxial tensile results of human valve cusps from a 20 y/o.[3] FSI simulations were performed by coupling FlowVision (Capvidia) with Abaqus/Explicit (Dassault Systems). Three cases were conducted from the TAV patient including (1) TAV, (2) virtual R/NC fusion with the same BCs to elucidate the impact of BAV alone, and (3) R/NC fusion with tuned BCs mimicking physiologic compensation to BAV. A validation case (4) included fusion from the R/NC BAV patient. Quantification of mechanical stimuli such as wall shear stress (WSS) and von Mises stress were then extracted.

Results: Virtual fusion of the R/NC cusps in case 2 revealed reduced systemic pressure requiring tuning of BCs in case 3 to match clinical values. Both R/NC BAV cases showed similar alterations in mechanical stimuli, with differences due to tuning of BCs. The fibrosa/aortic surface of the BAV experiences higher WSS on the noncoronary cusp compared to the fused cusp during systole. High magnitude von Mises stress is also present near the fusion site, which is not present on TAV cusps.

Conclusions: To our knowledge these are the first FSI simulations to characterize the mechanical stimuli for a young adult with R/NC BAV prior to calcification. The methods allowed for robust assessment of mechanical stimuli on the valve cusps, and thus may ultimately allow us to further characterize the temporal mechanical changes in pediatric BAV patients leading up to calcification.

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Personalized Computational Modeling Strategy to Simulate the Outcomes of Functional Mitral Regurgitation Repair Techniques

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Key Words: *Functional Mitral Regurgitation, Mitral Valve Repair, Modeling and Simulation, Finite Element Method*

Mitral valve (MV) is the left-sided atrioventricular valve of the heart, composed of the mitral annulus, two leaflets, branched network of chordae, and two papillary muscles. During systole, it prevents the retrograde blood flow between left ventricle and left atrium. Computational modeling of the MV has recently emerged from an approach used to define the native mechanics of the valve and explore its physiology and pathology, to a powerful tool that allows to investigate the impact of novel treatment strategies for the diseased MV. Several new techniques to surgically repair or replace the diseased valve are now in development. Therefore, patient-specific computational simulations of the MV function before and after surgical repair can help surgeons to assess the interventional outcomes of such repair techniques and may be extremely useful in preclinical procedure planning.

We report a patient-specific 3D echo-derived MV modeling strategy, which can assist in procedure planning for the repair of functional mitral regurgitation (FMR), a disease that alters MV geometry resulting in inadequate closure and backward leakage of the valve. Such strategy was developed using echo images obtained in pigs with FMR. For each collected dataset, images were segmented and finite element model of the MV was reconstructed. FMR was induced by pre-straining the chordae. Annular contraction and movement of the papillary muscles were set as patient-specific kinematic boundary conditions. Physiologic transvalvular pressure was applied on the leaflets and explicit dynamic finite element simulation of the MV closure was performed.

The results of our simulations faithfully mimicked MV alterations inherent to FMR: excess leaflet tethering and reduced mobility, restricted motion of the papillary muscles, increased interpapillary distance, elevated leaflet stresses and chordal tension forces. In addition, validation of the modeling strategy was performed by comparing computational results and imaging data: for each dataset, a good agreement between simulated configuration of the MV leaflets and corresponding 3D echo images was observed.

Furthermore, the developed modeling strategy was tested to investigate the outcomes of various FMR repair techniques: undersized mitral annuloplasty, papillary muscle approximation, and implantation of MitraClip and Cardiac Leaflet Enhancer (CARLEN). In each case, we acquired realistic and reasonable simulation results, comparable to the results obtained on the bench in our lab **[1]**,**[2]**. Therefore, the presented modeling strategy may be used for preclinical procedure planning to assess the outcomes of different FMR repair techniques.

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Statistical Shape Model of aorta and carotid arteries by using relative coordinates

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Key Words: *Statistical shape model, Hemodynamics, Deep learning, Data augmentation*

Deep learning has begun to be used for predicting hemodynamics instead of computational fluid dynamics (CFD) [1]. Deep learning is a data-hungry approach, yet obtaining enough number of medical data is difficult. Therefore, data augmentation plays an important role to maintain the accuracy of deep learning prediction. For 3D geometry of aorta, statistical shape model (SSM) is often used to increase the number of training data. SSM generates the virtual patient geometry using principal component analysis (PCA) of several real patient's geometry. However, in general, SSM has difficulty in maintaining the continuity of the geometry and controlling the geometry parameters. For these reasons, SSM is difficult to be applied to the complex artery shapes. In the study of artery SSM, only the aorta is mainly used [2]. In our study, we propose a new SSM approach for human's aorta with carotid artery parts.

The centerline and radius of each point was extracted from the 4 real patient's aorta and carotid artery STL data. The centerline of the aorta was divided into 30 equal parts. The carotid artery was also divided in the same span as the aorta. Virtual patient data was generated as a set of centerline for each artery part by SSM. Then, 3D surface was reconstructed around the centerlines. To maintain the continuity of the model, we used the relative coordinates of the centerline instead of the absolute coordinates. In the relative coordinates, the previous point was used as a reference. The vector from the previous point to the next point was represented as a coordinate value. To evaluate the continuity of the model, the angle between each point and the front and back points was calculated.

Our SSM successfully constructs both parts of aorta and carotid arteries. Since SSM was constructed independently for each artery part, deformation can be performed respectively. The average angle of the aorta part is 2.52 ± 0.52 rad in absolute coordinates. On the other hand, the average angle is 2.91 ± 0.18 rad in relative coordinates. From the value of the SD, there is a larger angle variation in the absolute coordinates. This result shows that SSM using relative coordinates maintains the countinuity of the centerline SSM.

Our developed SSM can add deformation to complex branches between aorta-carotid artery with maintaining continuity.

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A 3D Finite Deformation Continuum Model Framework for Active Synthetic and Biological Materials

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Key Words: *Hyperelasticity, Finite Element Model, Muscle Contraction, Shape Memory Polymers*

We develop a unified approach to mathematical modelling of muscles and polymeric 3D printed bionic actuators. It consists in three-dimensional finite element thermoelectromechanical modelling based on active strain approach. In the underlying mathematical model, the deformation gradient tensor is decomposed into passive and active parts. Passive response is modelled by a transversely isotropic nonlinear hyperelastic material model whereas the active behaviour is characterized by contraction associated with actin–myosin interaction in the case of muscles [1] or thermal activation in the case of polymers exhibiting shape memory (SM) effect [2].

In order to capture the SM effect, multi-branch models are often applied by considering the thermomechanical phase transition as the temperature crosses glass-transition temperature Tg. This type of models are time- and temperature-dependent and applicable for 4D printing with the fourth dimension referring to time [3]. 3D-printed SM polymeric objects demonstrate large recoverable deformations to the initial state being heated above Tg. Such programmable materials are often called “smart” due to their capability to change actively geometric configuration and widely used for medical, civil and aerospace applications.

Current research involves constitutive models for skeletal muscles and shape memory polymers revealing electromechanical and thermomechanical behavior respectively, three-dimensional finite-element implementation and the corresponding experimental investigations of SM behavior of 3D-printed polymeric objects.

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Effect of Lumbar Muscle Atrophy on Human Lumbar Intervertebral Disc Loading Change

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Key Words: *Muscle Atrophy, Intervertebral Disc Loading, Musculoskeletal Modelling*

Long duration spaceflight has been reported to elevate the rates of back pain and spinal diseases in astronauts. It has been observed that long-term microgravity exposure causes significant atrophy of lumbar spinal muscles [1]. Studies have reported associations between muscle atrophy and spinal diseases such as lower back pain and disc herniation. However, the biomechanical mechanisms underneath such associations are not clear. This study is aimed at exploring the influence of lumbar muscle atrophy on the loading of human lumbar intervertebral discs with a multibody modelling approach.

The effects of lumbar muscle atrophy on disc loadings were studied using a full body musculoskeletal model developed with the AnyBody Modeling system (AnyBody Technology,V7.3, Denmark)[2]. Specifically, the lumbar intervertebral discs were modelled as 6 degrees of freedom joints with linear elastic properties [3]. The swelling effects of the discs were considered, with swelling pressure dependent on the fixed charge density of the disc. The water content and fixed charge density are tissue deformation dependent. The ligaments were considered as non-linear elastic elements. The maximum strength of the muscles was dependent on muscle functional cross-sectional area (FCSA). In this study, atrophy of lumbar muscles was modelled with reduction of muscle FCSAs. Two levels of FCSA decrease, namely, 20% and 40% decrease, of lumbar muscle groups (multifidus, erector spinae, quadratus lumborum, psoas major, transversus abdominis, obliquus internus, and obliquus Externus) under eight daily postures (lying supine, slouched seating, straight seating, relaxed standing, standing bent forward, standing lifting a 20 kg weight close to chest, standing lifting 20 kg with spine flexed 45^{o}, and standing lifting 20 kg with arms stretched) were studied.

Our predicted loads on the lumbar discs under eight daily postures without muscle atrophy were consistent with experimental data [2]. The predicted compressive and shear forces on the lumbar intervertebral discs showed no significant change with lumbar muscle atrophy in lying and sitting postures. However, they increased in the standing and standing flexed postures with or without carrying weight. The degree of increase was larger at a higher level of muscle atrophy. This study is important for understanding the biomechanical mechanisms of how lumbar muscle atrophy may affect the lumbar intervertebral disc health.

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Machine Learning to improve Musculoskeletal Biomechanics Analysis

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Key Words: *Machine Learning, Neural Control, Personalization, Movement analysis*

We are currently researching the application of musculoskeletal (MSK) models for new goals, such as sports performance monitoring and prosthesis and exoskeleton design and optimization. These applications require advanced MSK models, for example personalized models, models that include a model of the neural control system, or real-time processing of measurements in the natural environment. MSK model personalization and model extensions are challenging, since invasive and/or expensive measurements are required, while real-time data processing, especially of measurement in the natural environment, requires new biomechanical data processing methods.

Machine learning (ML) is a promising technique to advance MSK models to achieve our goals. ML models could provide real-time data processing, while ML can also be used to extract more information from existing measurement data to allow for model personalization or extension. The application of ML has become possible recently due to the increasing availability of large datasets containing biomechanical movement data. Some laboratories have databases containing hundreds or thousands of measurements [1], while recent developments also allow for fast generation of movement simulations [2], which can artificially increase dataset size.

We currently investigate if and how combining MSK models and ML can advance MSK models towards our goals of sports performance monitoring and prosthesis and exoskeleton design and optimization. Therefore, we will present (preliminary) results and highlight future approaches where ML techniques are used to improve MSK model outcomes.

(1) **Machine learning for real-time biomechanical analysis in-the-wild.** We trained neural networks to output kinetics and kinematics from inertial sensor data, to develop an approach for real-time processing of biomechanical data recorded in the natural environment. We used gait simulations to increase data-set size and improve network accuracy [3].
(2) **Neural networks for gait control.** Currently, neural control models require a pre-defined model shape, e.g. a reflex model [4], which could bias their outcome. We are developing an approach to combine musculoskeletal simulations with neural network training to train unbiased controllers to replicate human control.
(3) **Personalized musculoskeletal models.** Gait measurements of each person are unique. Therefore, we will explore if we can train a neural network to personalize MSK models from gait measurements, and use these neural networks to investigate individual anthropometrics.

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Towards in vivo Passive and Active Force Estimation of Skeletal Muscle using Shear Wave Elastography

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Key Words: *Shear wave elastography, Biceps Brachii, Force Estimation, Electromyography*

Modelling and simulation of skeletal muscles are essential to better understand musculoskeletal diseases and improve treatment strategies. However model validation for in vivo muscular structures is not straight-forward. Muscle forces measured directly at the respective tendons intra-operatively can be used for validation [e.g. 1]. Though such an invasive intervention is not feasible for many scenarios in particular for healthy muscles. Surface electromyography (sEMG) is widely used for active muscle characterization, but it does not represent the passive state of muscles. Previously, muscle stiffness deduced from shear wave elastography (SWE) was shown to represent muscle mechanics [e.g. 2]. The objective of the present study was to investigate the use of a SWE approach in understanding active and passive force production of skeletal muscles in vivo by characterizing the biceps brachii muscle (BB) in relation to elbow joint position and function. We hypothesized that changes in mechanical properties of the BB can be detected both in passive state and during isometric ramp contractions at different activity levels for various muscle lengths. Therefore, we investigated whether SWE is a better method in revealing individual muscle mechanics in relation to joint function which would help improve existing muscle models.

SWE, sEMG of BB, and isometric elbow torque measurements were performed on 10 healthy volunteers (5 males, 27 ± 4.92 years, 72.7 ± 10.5 kg, 176.2 ± 5.03 cm) after they gave written consent to participate. A passive trial, maximum voluntary contractions (MVC) and isometric ramp contractions (up to 25%, 50%, 75% of MVC torque) were performed for five elbow angles (60°, 90°, 120°, 150°, and 180°).

At passive state, elastic modulus of BB deduced from SWE significantly changed between flexed and extended elbow angles (e.g. between 60°/90° to 180°, $p<0.02$) but no significant differences were observed for sEMG root-mean squared amplitude (RMS) ($p<0.05$), supporting our hypothesis of SWE but not sEMG being able to characterize passive mechanical muscle properties. During ramp contractions, we found that normalized sEMG represents muscle activity ($R^2>0.75$) but cannot detect contribution of BB to elbow function at higher lengths. In contrast to flexed positions, elastic modulus vs normalized elbow torque did not show a linear relationship at extended positions. We conclude that SWE providing more realistic results can be developed as an index of muscle force. If validated with experiments [e.g. 1], SWE findings can be used to improve muscle models and simulate the effects of e.g. exercise, neuromuscular conditions, or treatments.

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Understanding in vivo Skeletal Muscle Mechanics within Connective Tissue Matrix: An Intraoperative Approach

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Key Words: *muscle force, joint function, cerebral palsy, neurologic and non-neurologic foot deformities*

For a better understanding of human locomotion, it is necessary to relate individual muscle function to the joints it crosses. More importantly, it is essential to assess the mechanical behavior of skeletal muscles not only in isolation but also with respect to the connective tissue matrix that they are embedded in. Previously, we developed an intraoperative approach based on measuring muscle forces through its respective tendon using buckle force transducers during orthopedic surgeries [e.g. 1-3]. Using this method, the mechanical behavior of healthy and diseased hamstring muscles was investigated in relation to knee joint angle. We found that even though children were taken to surgery due to a severe knee joint limitation, the data collected from spastic hamstrings indicated no abnormal mechanical characteristics if the muscles are activated alone [1]. Interestingly, when activated together with antagonistic and/or synergistic muscles, systematic and significant increases of the muscle force were observed [2, 3]. These indicated the relevance of muscular interactions through connective tissues on joint restriction in neuromuscular diseases.

In the present work, force production capacities of muscles crossing the ankle joint are studied directly at various ankle positions. The experiments are performed in Universitätsklinikum Heidelberg, Germany after patients give written consent. The isometric forces of supramaximally stimulated triceps surae, tibialis anterior, and tibialis posterior muscles are collected at available ankle flexion and extension angles from patients with cerebral palsy, neurofibromatosis as well as non-neurologic foot deformities. Histological examinations performed on biopsied samples to quantify intramuscular connective tissue content are matched with the in vivo muscle function and state of the disease. The findings of the present study will reveal the effectiveness of surgeries performed in order to improve foot deformities such as tibialis anterior or tibialis posterior tendon transfers where not only the tendons but also the fascial connections are disrupted. The results will be discussed in terms of improving the existing modeling and simulation approaches that aim to guide surgical decision making and treatment strategies. In combination with advanced marker-based motion tracking and ultrasound imaging as well as MRI scans obtained before and after surgery, a 3D continuum-mechanical model based on unique constitutive laws will be possible.

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Whiplash Simulation: How Muscle Modelling and Movement Interact

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Key Words: muscle, eccentric contraction, impedance, titin, crash simulation

Whiplash injury and associated disorders are costly to society and individuals. Accurate simulations of neck movement during car accidents are needed to assess the risk of whiplash injury. Existing simulations indicate that Hill-type muscle models are too compliant, and as a result, predict more neck movement than is observed during *in-vivo* experiments.

Simulating head and neck movement is challenging because many of the neck muscles operate on the descending limb of the force-length curve [1], a region that Hill-type models inaccurately capture. Hill-type muscle models have negative stiffness on the descending limb of the force-length curve and so develop less force the more they are lengthened [2]. Biological muscle, in contrast, can develop large transient forces during active lengthening and sustain large forces when aggressively lengthened [3].

Recently, a muscle model has been developed [4] that mimics the active impedance of muscle in the short range and can capture the large forces generated during extreme lengthening. In this work, we will compare the accuracy of simulated neck movements, using both a Hill-type model and the model of Millard et al. [4], to the *in-vivo* neck movement. If successful, the improved accuracy of our simulations will make it possible to predict and help prevent neck injury.

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Cleft palate treatment for late patients – a study on simultaneous distractor application as an improvement on traditional orthodontic procedures

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Key Words: *Dental Biomechanics, Cleft Palate, Finite element simulation*

Cleft palate patients can significantly benefit from treatment based on alveolar graft deposition, a procedure with high success rate in young people. When treatment is delayed, after 12 years of age, the success of the procedure drastically decreases [1]. Probable causes for this decrease in success is the absence of both the child's growth stresses in the maxilla as well as of the eruption of the second dentition, which occurs up to the age of 12 [2]. This study aims to use numerical simulation to analyse the effect of a distractor to enhance the results of alveolar graft treatment in late cleft palate patients. The process of expanding the maxilla simultaneously with graft deposition would ideally induce stresses in the bone graft region, leading to osteoblast activation and bone growth.

After standard cleft palate treatment without distraction, cone-beam computed tomography (CBCT) images were compared to a numerical simulation. The linear elastic model with non-homogeneous elastic moduli for the bone was subjected to a loading simulating palatal expansion using the distractor in ANSYS. The patient's graft density data were correlated to the bone elastic modulus to simulate the clinical conditions of maxillary expansion. Graft density data were acquired from CBCT images and loaded into automated reconstruction commercial software Dolphin 3D and the geometric model was constructed in MIMICS.

The comparison of MEF stress distribution with the clinical bone resorption images of the CBCT for a cleft palate adult patient 60 days after surgery showed that low stress levels in the middle of the graft coincided with graft reabsorption areas as expected. As for the simulation of the use of the distractor simultaneously with the graft application produced evidence that the stress distribution corresponds to a situation that can be related to a positive stimulus to bone growth and graft consolidation. Further clinical research is needed to validate these results, and numerical simulation has shown its potential for guiding alternatives in cleft palate treatment.

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Computational cardiac electromechanics: the role of mechano-electric feedback and its arrhythmogenic effects in three-dimensional ventricular models

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Key Words: Cardiac electromechanics; Mechano-electric feedback; Stretch-activated channels; Commotio cordis; Precordial thump; Premature ventricular contraction

The role of the human heart is to circulate the blood in order to provide every cell with vital nutritions via the cardiovascular system. Any irregularities might lead to the loss of life quality, and even sudden death. Therefore, stable circulation in the cardiovascular system is important. The steady and healthy circulation can be performed by the well-balanced harmonization between Excitation Contraction Coupling (ECC) and Mechano-electric feedback (MEF). In contrast to ECC, by which electrical activation of cardiac cells triggers the mechanical contraction of the heart, is well characterized, less is studied about the cellular mechanisms of MEF, where mechanical alterations in the heart influence back cardiac electrical activity.

The goal of this study is to investigate the role of MEF in healthy cardiac cycles and in cardiac arrhythmia using human ventricular models. The effect of MEF is manifested by stretch-activated channels (SACs). The numerical formulation of SACs in terms of the fibre stretch of the myocardium is embedded in the modified Hill model that describes the myocardium as an electro-visco-active material [1]. In addition to the existing models of SACs in terms of the stretch along fibre direction [2], we propose models of SACs formulated in terms of the rate of stretch along fibre direction and the stretch along sheet direction. The influences of the three different models for SACs and different material properties on the regular cycles are analyzed by using the electrocardiogram and volume-time curves, and show that the each model of SACs leads to regionally varying reactions on the heart model. Moreover, we simulate 'commotio cordis' and 'precordial thump' and demonstrate that MEF take a vital role in fibrillation and defibrillation without the structural impairment in the heart. Furthermore, we study the role of MEF in premature ventricular contraction when the heart is hemodynamically disturbed.

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Fractional Viscoelastic Modeling of Cardiovascular Soft Tissues

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Key Words: Biomechanics, Constitutive Modeling, Viscoelasticity, Fractional Derivatives, Cardiovascular Tissues

While experimental evidence shows that the mechanical response of most tissues is viscoelasticity, current biomechanical models used in computational studies often assume only hyperelasticity. Fractional viscoelastic constitutive models have been successfully used in literature to capture the material response. However, the translation of these models into computational platforms remains limited due to a computational cost that is $O(N_T^2)$ and a storage cost that is $O(N_T)$ in order to store and integrate historical data. We developed a novel numerical approximation to the Caputo derivative which exploits a recurrence relation to give a computational cost that is $O(N)$ and a storage cost that is fixed over time [1]. We used this approach to extend the conventional analysis of residual stress in aortic soft tissues by considering the effects of viscoelasticity [2]. A substantial portion viscoelastic tissue is necessary to capture the long-term dynamics of the residual stress experiment. In addition, the results show that conventional estimates of residual stress are over-estimated a factor of 2 and that viscoelasticity is necessary to accurately estimate residual strain. Using this approach, we developed a fractional viscoelastic model for myocardium that improves the quality of fit compared to current models in the literature [3]. This allows us to develop an inverse modeling approach, incorporating full 3D fiber architectures, for the estimation of the viscoelastic properties of myocardium from tri-axial mechanical experiments. These results demonstrates that fractional viscoelasticity has enormous potential for facilitating the analysis of viscoelastic properties of soft biological tissues in computational problems.

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Modeling the two-pathway contraction of smooth muscle in arterial walls

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Key Words: Biomechanics, Arterial Wall, Smooth Muscle Cells, Active Response

Patient-specific numerical simulations are considered a promising toolbox for the improvement of clinical practice by allowing the detailed numerical analysis of atherosclerotic arteries with respect to e.g., efficiency and influence of antihypertensive drugs or plaque development and rupture. One important contributor influencing the resulting mechanical fields is the active contraction of smooth muscle which is in turn influenced by the deformations due to a change of the intravascular pressure. During the stretch of smooth muscles cells (SMCs), two different mechanisms are triggered: the calcium-dependent and the calcium-independent contraction [1]. For the calcium-dependent contraction mechanism, the stretch of the SMCs leads to an inlet of calcium ions through various different pathways and activates the myosin light chain kinase (MLCK) leading to the contraction. For the calcium-independent contraction mechanism, stretch-dependent receptors of the cell membrane stimulate an intracellular reaction chain which leads to an inhibition of the antagonist of MLCK, the myosin light chain phosphatase (MLCP). While the calcium concentration can change over a rather small time frame, the inhibition of MLCP lasts much longer. We present a chemo-mechanical model which describes both, the calcium-dependent and the calcium-independent contraction of SMCs. As a basis for the mechanical description of the contractile units, the model by Murtada et al. [2] making use of the chemical model of Hai and Murphy [3] is considered. A new set of equations is presented to describe the stretch-dependent calcium inflow and the inhibition of MLCP as a contractile mechanism. An algorithmic framework for the implementation of the model in finite element programs is derived. Based thereon, simulation results of arteries under time-dependent intravascular pressure, mimicking the scenario during a heart-beat, are analyzed and the influence of the proposed model is shown. Quantitative comparisons with experiments show that the response of the model enables realistic numerical simulations.

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Validation of FEM-based patient-specific knee joint motion simulation

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Abstract

Knowledge about patient-specific knee joint dynamics is crucial for the decision on therapeutic options in order to restore stability and functional/physiological joint motion after a cruciate ligament rupture. To achieve best possible approximation to the patient's native pre-traumatic knee joint condition, our research focus is concerned with a dynamic three-dimensional knee joint model employing the Finite Element method (FEM) for the assessment of the individual biomechanics. The patient-specific FE-model is automatically generated based on MR image segmentations of relevant anatomical structures of the knee joint: bones, articular cartilages, menisci, and ligaments. Linear and non-linear constitutive models, including initial strains are considered for modelling soft tissues. MR measurements of volunteers with in-situ loading (flexion, internal and external rotation) were used to validate the kinematics of bones and menisci. Analyses of simulation results as well as comparisons to MR measurements at selected flexion and rotation angles are shown in Figure 1. The simulated patient-individual knee joint biomechanics can be used in the decision process in order to restore stability and physiological joint motion after a cruciate ligament tear. Our vision is to establish computer-assisted ligament reconstruction planning in clinical routines.

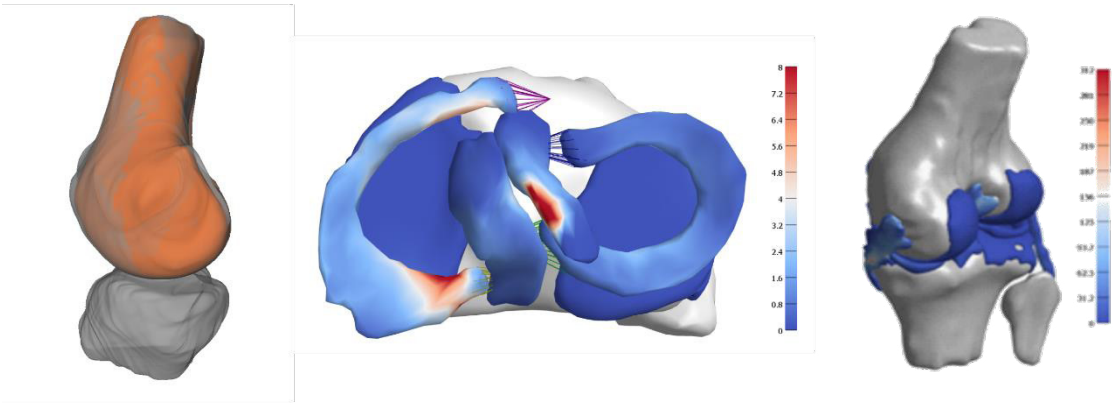

Figure 1: FEM-simulation of a knee joint up to 20° flexion with subsequent external rotation up to 28° and the corresponding stresses [MPa]. Left: comparison of simulation-based femur position (orange) with MR measurement (grey). Middle: meniscus and cruciate ligament dynamics at external rotation. Right: dynamics at external rotation.

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A Numerical Investigation of the Membrane Tensions and Motional Behaviors of Circulating Tumor Cells in Microvessels

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Key Words: *blood flow, circulating tumor cell, membrane tension, cell dynamics, hemodynamics*

The membrane tensions of suspended nucleated cells moving in blood flows in microvessels are quite different from those of spreading cells, which is crucial to many pathological processes, such as the metastasis of cancers via circulating tumor cells (CTCs)[1-3]. However, few studies have examined membrane tensions in suspended cells, especially when interacting with other cells of different stiffnesses in low–Reynolds number flows at the cellular level. Taking CTCs as an example, we use the immersed boundary method to analyze the relationship between membrane tensions and their motional behaviors under the influence of fluid–cell–vessel interactions. The effects of vessel diameter and hematocrit on the shear tension and average isotropic tension are also analyzed. The results suggest that the confinement of the vessel wall determines membrane tensions on CTCs until the ratio of the vessel diameter to cell size becomes slightly larger than unity, at which point cell–cell interactions become the crucial factor. The increase in interactions between red blood cells (RBCs) and CTCs with the increase in the hematocrit in larger vessels promotes membrane tensions not only through the migration of CTCs to the vessel wall but also through a reduction in the translational motion and rotation of CTCs. The present study provides support rooted in biofluid mechanics for mechanobiological research on the metastasis and apoptosis of CTCs in microvessels.

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A Numerical Study on the Effects of Mechanical Properties of Red Blood Cells on Rheology in Narrow Microchannels

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Key Words: *Narrow Channel, Large Deformation, Buckling, Fluid-Structure Interaction*

The changes of the mechanical properties of red blood cells including the ratio of surface and volume, and shear modulus affect their dynamical behaviours in microcirculations apparently, and the interaction of cells and their surrounding fluid has a critical impact on the design of microfluidic chips as well. Here, we investigated the large deformations of a single red blood cell in extreme narrow channels and the hydrodynamics associated. The cell membrane was modelled as a hyper-elastic thin shell. The cytoplasm was treated as Newtonian fluid with larger viscosity than the outer fluid. The immersed boundary method was adopted for the fluid-structure interaction. Strict conservation of the surface area and volume of cell were achieved.

Numerical results show that the flow resistance correlates with the capillary number in two different mechanisms. At a relatively high capillary number (> 0.2), the average thickness of the thin film between the cell membrane and the vessel wall dominants flow resistance approximately following lubrication theory. At a relatively small capillary number (< 0.1), cell membranes often present wrinkles, at which the flow resistance is higher than that predicted with lubrication theory. This deviation is due to the inhomogeneous distribution of outer fluid vorticity around the membrane. By increasing the reduced volume of the cell, the wrinkles and the resistance deviation from lubrication theory decrease.

The present study helps in understanding the discrepancy in measure the mechanical property of single cell with narrow channels.

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Data Assimilation Method for Estimating Membrane Permeability Based on the Langrange Multiplier Method: Formulation and Fundamental Examination

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Key Words: *Data Assimilation, Membrane Permeability, Lagrange Multiplier Method, Finite Element Method*

Mass transfer phenomena across biological membranes can be observed everywhere in the human body. Erythrocytes in a blood supply oxygen to cells through the erythrocyte membrane and blood vessel walls. It has been reported that atherosclerosis is caused by the accumulation of low-density lipoproteins under the vascular endothelium. Quantitative methods to measure the permeability of biological membranes are required for further understanding of biological activities in the body and elucidation of circulatory disease mechanisms. As a computational technique using measurement data, the data assimilation method have often been used to improve the accuracy of the data or to estimate unknown parameters. For hemodynamics application, D'Elia et al. proposed a data assimilation method that minimizes the difference between the computational fluid velocity obtained from the steady Navier-Stokes equations and the measured velocity data. In this study, following the concept of D'Elia et al's study, we propose an estimation method for the membrane permeability such that the concentration distribution from the diffusion equation and the measured concentration data are minimized. The diffusion equation with the transport equaiton of the membrane was formlated as the weak form. The equation was descretized using the finite element method, and a minimization problem was set up to minimize the difference in concentration between experiment and calculation using the Lagrangian multiplier method. The system of equations was derived from the stationary condition and the solution was obtained numerically. In order to verify the proposed method, one-dimensional problem was set up. The proposed method was applied to artificial concentration data with noise, and it was confirmed that the proposed method can estimate reasonable values of the membrane permeability coefficients.

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Deformation Mechanics of a Red Blood Cell under Shear Flow

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Key Words: *Biomechanics, Red Blood Cell, Cell Membrane, Viscoelasticity, Boundary Element Method, Mechanical Testing*

Determining the viscoelasticity of a red blood cell (RBC) is important in understanding its mechanics, which can be used to monitor health. Under strong shear flow, elongation deformation of an RBC accompanying a tank-treading (TT) motion increases with fluid shear stress relative to the membrane's viscoelastic stress. Here, the RBC deformation was numerically simulated to understand its mechanical characteristics. The boundary element method was used to couple the viscoelastic deformation of the cell membrane and viscous flow of the surrounding fluids. As a result, deformation and inclination angle of the RBC were related to the fluid traction difference between the suspending and RBC inner fluids [1]. When the viscosity of an RBC is compatible with the suspending fluid, the elongation index responding fluid shear stress is similar to the responding external loads in the optical tweezers stretch, but elongation mechanics differed. By identifying the viscoelasticity of the cell membrane to reproduce published experimental data, the strain hardening elasticity of the cell membrane was identified by modifying the model developed by Skalak et al. [2]; the exponential form of Fung [3] successfully expressed the stronger strain hardening behavior for the latter deformation regime. These results indicate the applicability of the shear flow experiments as a stretch testing method to measure the viscoelasticity of the cell membrane.

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Effects of Geometrical Alteration on Left Atrial Hemodynamics after left upper lobectomy

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Key Words: *Left Atrium, Pulmonary Vein, Hemodynamics, Computational Fluid Dynamics*

Computational approaches to express left atrium (LA) hemodynamics are potentially useful to diagnose LA thrombosis. Recent cohort studies[1] clarified that left upper lobectomy (LUL) with left superior pulmonary vein (LSPV) resection in thoracic surgeries has a higher prevalence of LA thrombosis. Because PV geometries have large patient-specific differences and relative posture of the remaining PVs can be altered by the lobar resection, alteration of the remaining PVs posture after the LUL may affect the LA hemodynamics. This study aims to evaluate the impact of the remaining PVs geometric alteration on LA hemodynamics after the LUL using 4D-CT based computational fluid dynamics simulation.

4D-CT images (20 phases/cardiac cycle) for three lung cancer patients before and after the LUL were acquired in Jichi Medical University hospital. LA surfaces were reconstructed from 4D-CT images and these displacement field were estimated by a non-rigid point registration[2]. Computational simulations of the LA blood flow were conducted by solving the incompressible N.S. equation with the prescribed LA moving-wall boundary condition in a finite difference manner. The wall boundary conditions were treated by the boundary data immersion method[3]. For each patient, we conducted blood flow simulation before and after the LUL. Moreover, we computed an artificial LUL case, in which the LSPV is artificially resected from preoperative geometry to focus on the effects of LSPV resection without changing relative postures of the remaining PVs on the LA hemodynamics.

Obtained results showed that jet flows from each PV into the LA in almost whole cardiac cycles in every case and these jets much progressed in cases with artificial LSPV resection comparing to preoperative case. While after LUL, the collision regions of jet flows changed due to the alteration of the jet flows direction. These findings suggest that the alteration of LA hemodynamics was not only induced by the LSPV resection, but also the alteration of atrial and remaining PV anatomies by the LUL.

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Numerical analysis of equilibrium state and lateral migration of erythrocytes in 3D cylindrical microchannel

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The steady motion and equilibrium location of red blood cells (RBCs) in microchannels is a key issue in cellular-scale hemodynamics and microfluidics. However, full information of the dynamic behaviors of cells in 3D circular tubes to varied flow conditions is lacking. We investigated the dynamic behavior of erythrocytes across a wide range of flow rates and beginning locations in order to obtain phase diagrams of the equilibrium state. When shear rates are low ($\dot{\gamma}^* < 0.1$), the equilibrium state of the cell shifts from "Snaking" to "Tumbling", then "Slipper" to "Parachute." For high shear rates ($\dot{\gamma}^* > 0.1$), the equilibrium state of a cell may be either "slipper" or "parachute," depending on its starting position. While both of these factors affect the deformability of erythrocytes, shear modulus has no effect on the pattern of equilibrium state and position, whereas the ratio of internal to external viscosities decreases, and the equilibrium state tends to become "Snaking" or "Parachute" near the tube center. Due to the difference in beginning locations, an erythrocyte's equilibrium state might be "parachutes" or "slippers," with "slipper" erythrocytes traveling quicker and having less membrane tension. Not only does this work provide light on mass transfer mechanisms influenced by RBC dynamic behaviors in microcirculation, but it also paves the way for the development of efficient microfluidic chips for cell sorting.

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Numerical analysis of the lateral movement of red blood cells in circular microchannels

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Key Words: Axial migration, red blood cell, Newtonian fluid, circular channel flow

Human red blood cells (RBCs) are subjected to high viscous shear stress, especially during microcirculation, resulting in stable deformed shapes such as parachute or slipper shape. Those unique deformed RBC shapes, accompanied with axial or nonaxial migration, cannot be fully described according to traditional knowledge about lateral movement of deformable spherical particles [1]. Although several experimental and numerical studies have investigated RBC behavior in microchannels with similar diameters as RBCs [**?**], the detailed mechanical characteristics of RBC lateral movement–in particular, regarding the relationship between stable deformed shapes, equilibrium radial RBC position, and membrane load–has not yet been fully described. Thus, we numerically investigated the behavior of single RBCs with radii of 4 μm in a circular microchannel with diameters of 15 μm or more. The problem was characterized by Reynolds number and the capillary number Ca, which is the ratio between fluid viscous force and membrane elastic force. The power (or energy dissipation) associated with membrane deformations was introduced to quantify the state of membrane loads. RBCs, modelled as biconcave capsules whose membrane follows the Skalak constitutive law [2], is simulated for a wide range of viscosity ratios between the cytoplasm and plasma, for different Re and Ca. Since this problem requires heavy computational resources, we resort to graphics processing unit computing, using the lattice-Boltzmann method for the inner and outer fluid and the finite-element method to follow the deformation of the RBC membrane. Simulations were also performed with different initial RBC centroid positions. Our numerical results demonstrated that, especially for almost inertialless, axial or nonaxial migration of RBC depended on the stable deformed RBC shapes, and the equilibrium radial position of the RBC centroid correlated well with energy expenditure associated with membrane deformations.

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Quantitative Prediction of Rolling Dynamics of Leukocyte-inspired Microroller in Blood Flow

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Key Words: *Blood cells, Bio-inspired microroller, Rolling dynamics, Drug delivery, Mesoscale modelling*

Magnetic microroller, inspired by leukocyte in the microcirculatory system, represents a promising candidate for targeted drug delivery [1,2]. However, the rolling dynamics of individual microroller in response to controlled changes in shear stress and magnetic field remains largely unknown. Here, we develop a mesoscopic model of the leukocyte-inspired microroller to investigate its locomotion behaviour inside blood vessel under different shear stresses and magnetic torques. We find that the microroller can roll along with the blood flow or move against the bloodstream depending upon the competition between applied magnetic torque and fluid shear stress. Our simulations reveal that the microroller can achieve precise navigation under low shear stress levels. We also probe the effect of blood haematocrit on the dynamic performance of the microroller, which shows that the shear-induced collisions between erythrocytes and the microroller can significantly alter the motion of the microroller, especially under high haematocrit levels. In addition, we examine the rolling dynamics of the leukocyte-inspired microroller in a bifurcating microfluidic channel, demonstrating that the microroller can navigate along the user-defined path. These findings provide unique insights into the rolling dynamics of individual microroller in physiologically relevant blood flow, and offer an objective way for facilitating the design of bio-inspired microrollers in targeted and localized therapeutic delivery with high precision and efficiency.

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Study on flow behaviors of hemoglobin-based oxygen carriers through microvessels

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Key Words: *Red blood cells, Hemoglobin-based carriers, Lattice Boltzmann method*

Various types of hemoglobin-based oxygen carriers (HBOCs) are currently being developed as transfusion alternatives for solving chronic blood-supply shortage issues arising from rapidly declining birth rates and aging populations. These carriers are also essential for reducing the inherent risks associated with current blood preparation proceses. For example, cellular Hb vesicles (HbVs) that encapsulate the concentrated Hb solution in phospholipid vesicles are being vigorously promoted in Japan and have been recognized as useful alternatives for red blood cells (RBCs). The diameter of typical LEH particles ranges from approximately 200 nm to 250 nm, which is roughly 1/30th the size of a human RBC. Thus, the effect of HbVs will be significant at a microcirculation level, where vessel diameters are smaller than the RBC diameter. Studies focused on RBC and HbV flow distributions at this level will elucidate the effect of HbVs on organ perfusion and tissue oxygen delivery. Therefore, in the present study, the behaviors of flow with mixed RBCs and HbVs in microvessels were analyzed.

In the present study, we adopt the lattice Boltzmann method (LBM) for the computation of flows. The LBM is a relatively new and promising numerical scheme for simulating complex flows and has attracted considerable attention as an alternative approach to conventional Navier-Stokes equations for computational fluid dynamics. One advantage of the LBM is the simplicity of handling complex moving geometries. Therefore, LBM is very effective for the analysis of multiphase fluid flows (for example, those considered in the present study). We treated the RBC membrane as a neo-Hookean model. In this study, we employed the immersed boundary method (IBM) to examine the fluid-membrane interaction between the flow field and deformable RBCs.

In conclusion, the present LBM simulations revealed the flow behaviors of RBC and HbV at a microvascular bifurcation. The partial replacement of RBC by HbV reduces the bias of the oxygen flux. The present result suggests that HbV contributes to reducing the heterogeneity of the oxygen supply, possibly improving the oxygenation of ill-perfused regions. Further numerical analyses based on the arterial-capillary network are needed to clarify the overall effect of HbV transfusion on organ perfusion.

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Clinical Relevance: the Key Motivator in Designing and Conducting Computational Studies of the Shoulder

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Simulations of the rotator cuff (RC) have the potential to be used to enrich our understanding of the mechanical environment of the tendon and inform clinical decision-making. For these simulations, the ultimate goal is to build a framework that can be used by clinicians to support recommendations for their patients and ultimately improve the patient's quality of life. The clinical translation of such a framework depends on the synthesis of data from a myriad of sources to achieve a useful and accurate clinical recommendation. The ideal framework will be patient-specific, including tendon status and material properties, motion-specific and adaptable to the activities and activity level of the patient, and will use a validated method for estimating the mechanical environment of the RC to estimate tear initiation and progression risk. The framework will also consider the biological and other potential confounding factors that affect the mechanical environment of the RC tendons. To achieve clinical utility, the framework requires feedback from clinicians, ideally comprehensive long-term patient assessments that can be used to quantify the quality of the initial recommendations. The final stages of this framework will provide clear and concise, quantified clinical recommendations easy for the clinician and the patient to understand and to act on. The field has not yet achieved a mature, clinically translatable simulation framework, but the foundation for many of the pillars that this future ideal framework will rely heavily on have recently been built. Through iterative collaboration between scientists and clinicians, we will build clinically effective simulations that will enhance our understanding of RC tear pathomechanics and pathophysiology to ultimately improve patient care.

Therefore, we propose a round table made up of clinicians and scientists evaluate and offer a framework for improved clinical relevance.

Finite Element Model of Articular Sided Rotator Cuff Tear

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Key Words: *Finite Element Modelling (FEM), Rotator Cuff Tear (RCT)*

Introduction:

Rotator cuff tears (RCT's) occur in about 22% of the population over 50 years old, with the prevalence increasing as age increases [1]. Among those with RCT's about 65% of tears are asymptomatic [1]. Of patients that have asymptomatic RTC's, 36% will develop symptomatic RTC's within three years [2]. With the population expected to double for the 65–85-year-old population by 2050[3], it is increasingly important to tear progression. The aim of this study is to use Finite Element Modelling (FEM) to better understand the strains the supraspinatus experiences for an articular sided partial tear.

Methods:

To model partial tear on the supraspinatus, a validated FEM of an intact tendon first most be contructed. The articular and bursal side of the supra spinatus will be split to account for the varying material properties on each side. Each side will then be futher split into subsections to define the heterogenous material properties of the supraspinatus. The supraspinatus will be constrained for no translation or roation at the tendon insertion site of the greater tubercle of the humeral head and pulled to 4.14mm to match the conditons applied to a cadaveric study that was conducted to measure surface strain of the articular and bursal side of the supraspinatus. The strains will be compared to validate the FE model. To simulate partial tear, a new boundary condition will be applied where only the bursal side of the tendon insertion site is contrained.

Results:

The model was validated within a maximum of a 3% strain difference between articular and bursal X and Y principle strains when compared to the cadaveric data. The strain from the FEM of partial tear showed the same strain when the tendon ensertion was completely connected.

Discussion:

The goal of this study was to create a validated FEM to be used to model partial rotator cuff tears to better understand the strains associated with tears to help elucidate tear initation and propagation. Our initial findings indicate no differences in strain when the articular sided insertion of the tendon is not constrained. The next steps are to make a more refined model that includes the infraspinatus and give regions close to the inrestion zero stiffness to replicate tears and assess strain differences. These findings may help to better understand the onset of tears by evaluating the strain differences between a partially torn and a healthy tendon.

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Influence of Implant Design, Placement, and Soft Tissue Restraint Upon Shoulder Mechanics after Reverse Shoulder Arthroplasty

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Key Words: *Reverse Shoulder Arthroplasty, Post-impingement Instability, Dynamic FEA*

Combinations of implant design elements, positioning, and soft tissue tensioning are used to improve pre-impingement range of motion (ROM) and stability after reverse shoulder arthroplasty (RSA). However, RSA patients may occasionally undergo motions beyond impingement.

We implemented a dynamic, explicit FE model of RSA validated against experimental contact pressure during scapular impingement [1]. Bony (scapula, humerus) and soft tissue (subscapularis, deltoid) geometries were acquired from Visible Human CT scans. Bone and glenoid components were modeled as rigid, while soft tissues, polyethylene liner, and the bony scapular impingement region were modeled as deformable. Contact was defined at all relevant interfaces. Soft tissues were tensioned and wrapped around the joint/implant prior to motion. With the scapula fixed, humeral rotations were prescribed about anatomic axes. The mechanical trade-offs associated with various implant design features, placement, and subscapularis restraint/quality were investigated.

Increasing glenosphere lateralization increased impingement-free ROM, but the deltoid force required to elevate the arm [2] and the torque required for external rotation [3] also increased. Presence of the subscapularis was found to restrain post-impingement instability [4]. However, external rotation torque increased with increases in subscapularis stiffness [3]. In general, absence of the rotator cuff musculature produced greater impingement likelihood and post-impingement instability. Placing the glenosphere in neutral version together with rotating the liner posteriorly resulted in the greatest post-impingement stability [5]. While providing greater stability during abduction, a valgus angle of inclination liner design resulted in greater post-impingement instability during external rotation and extension, made worse by the absence of the subscapularis [4].

Simulating the full range of functional activities, while incorporating soft tissue tensioning and restraining effects, may aid in preoperative planning to improve pre- and post-impingement stability and overall outcomes after RSA.

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A Computational Biomechanical Model of Infant Triceps Surae Muscles Generated from Comprehensive Digitized Fascicles

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Key Words: *Paediatric, Musculoskeletal Modeling, Digitized Fascicles, Finite Element*

This research aims to develop a computational workflow to create paediatric musculoskeletal finite element models to understand infant muscle biology and mechanics. Muscle fibre fascicles (FFs) and connective tissues were digitized in a 6-month-old female cadaver; TS muscles were outlined from origin to insert attachment sites and digitized using a MicroScribeTM G2X Digitizer (0.05 mm accuracy; Immersion Corporation, San Jose, CA). The digitized data were used to create qualitative 3D muscle models in Autodesk® Maya® [1]. Fascicles of each muscle were wrapped by 2D convex skin grids and then converted into volumetric tetrahedral meshes. Information from fibre fascicles was used to define the fibre orientation as inputs for a Transversely Isotropic Mooney Rivlin material property in a finite element model. The FE model was set in FEBio (Salt Lake City, UT, USA); model parameters were tuned to reproduce the passive range of motion of in vivo and cadaveric experiments [2]. Lagrange strain was computed from the incremental applied load (200N) at the calcaneus bone to mimic antagonist ankle dorsiflexion loading. Maximum strains were observed at the myotendinous junctions of the muscles, and non-uniformity of stress and strain patterns were observed, suggesting that there are local inhomogeneities of mechanical strains and biological remodelling of these tissues. To reach the maximum passive dorsiflexion, nearly 80%, 50%, and 10% strain were observed in lateral gastrocnemius, medial gastrocnemius, and soleus. We developed robust computational modelling (converging time <1min with single CPU) to map the stresses and along-fibre strains in triceps surae muscles, suggesting rapid muscle remodelling in origin and insertion regions of the muscle. Future work will continue digitizing more specimens to create a statistical shape modelling of paediatric TS muscles and develop a real time surrogate TS muscle musculoskeletal model applicable in clinics. This work is a step forward in development of biomechanical models from high fidelity anatomical data.

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Coupled Machine Learning and Finite Element Analysis of Heart Left Ventricle in Patients with Cardiomyopathy

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Key Words: *cardiomyopathy, heart left ventricle, machine learning, 3D reconstruction*

Automatic diagnosis of dilated cardiomyopathy based on ultrasound images is a challenging task, because pixel intensity levels in the images are not related to the physical properties of the tissue, as well as there is poor signal-to-noise ratio in images and weak echoes. Therefore, this study develops an automated methodology for 3D reconstruction and analysis of heart ventricle (LV) in patients with cardiomyopathy that can be divided into three main steps: (1) machine learning algorithms to extract LV and relevant parameters, (2) geometrical algorithms to reconstruct 3-dimensional model and (3) finite element method to analyse the mechanical response of the left ventricle under different loading conditions. Collected dataset consisted of 1809 images with apical view and 53 images with an M-mode view from cardiomyopathy patients at clinical facilities in the United Kingdom and Serbia. Methodology for analysis of apical view was based on segmentation of LV using U-net convolutional neural network [1] after which the segmented region was bounded with rectangle, where the longer side corresponds to left ventricular length (LVL). Regarding the M-mode view, traditional algorithms such as adaptive histogram equalization, template matching, Canny edge detection, and thresholding are used to extract internal dimension (LVID), posterior wall thickness (LVPW), and interventricular septum thickness (IVS), due to the smaller number of images. When manually annotated and automatically extracted parameters are compared, a dice coefficient of 92.091% for segmentation is obtained, as well as an average root mean square error (RMSE) of 0.3052cm for parameter extraction in apical view images and an average RMSE of 1.3548cm for parameter extraction in M-mode view images. Based on extracted left ventricle length, radiuses, wall thicknesses, and user-supplied divisions, 3D parametric model of LV is reconstructed, which can be used to replicate the entire cardiac cycle using Finite element method (FEM). Described methodology is integrated into SILICOFCM platform [2]. Fully automated cardiomyopathy identification, 3D reconstruction, and cardiac cycle modeling of the left ventricle utilizing ultrasound pictures can assist doctors in making more timely judgments and establishing more accurate therapies. The approach is now available on a user-friendly platform in order to help clinicians make faster decisions and establish reliable treatments.

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Membrane Left Ventricle Model Generated from Echocardiography

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Key Words: *echocardiography, left ventricle, membrane finite element, cardiac cycle.*

One of the very effective tools for tracking the cardiac cycle is echocardiography. This technique helps doctors to assess the heart function of a patient. Echocardiography is the most commonly applied technique for non-invasive assessment of cardiac state. In this paper, we presented the semi-automatic generation of the solid left ventricle model based on the images acquired from echocardiography. We generated model from the echocardiographic image at the start of diastole. Starting from there, we prescribed displacements using models generated at other time instances of the echocardiographic data. Since the dominant stresses lie in the sheet planes, while normal stresses in the wall normal directions are of the order smaller, we explored a possibility to model heart wall by membrane finite elements, hence considering the wall as a thick membrane (shell without bending effects). The membrane element is composite, containing layers over the thickness and variation of the direction of fibers. The membrane elements enables us to simulate heart mechanics which are much smaller and simpler for use than conventional 3D models. As a material model, we used the recently developed computational model [1] based on Holzapfel experiments [2,3] for the determination of passive stresses within cardiac tissue. The presented approach of modeling mechanics of the LV can serve as the basis for practical applications since it is based on the true patient-specific geometry and relies on experimental constitutive relationships.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Computational Modeling of Fingering in Stretched Hydrogel Cylinders

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Key Words: Fingering, Elastic Instabilities, Finite Element Method, Hydrogels, Soft Matter.

Recent experiments on hydrogels subjected to large elongations have shown elastic instabilities resulting in the formation of geometrically intricate *fingering* patterns. In this talk, we present a robust computational framework to simulate this complex material response from the onset of instability to the post-bifurcation behavior. We discuss the numerical challenges stemming from the non-convexity of the strain energy density in the near-incompressible, large-deformation regime, which is responsible for the coexistence of multiple equilibrium paths with vastly-different, sinuous deformation patterns immediately after bifurcation. We show that these numerical challenges can be overcome by using high order of interpolation in the finite element approximation, an arc-length nonlinear solution procedure following the equilibrium path of the system, and a parallel implementation enabling large-scale simulations. The resulting computational approach provides the ability to conduct highly-resolved, truly quasi-static simulations of complex elastic instabilities. Finally, we present numerical results demonstrating the ability of the path-following approach to describe the full evolution of fringe and fingering instabilities observed experimentally. Importantly, we observe that the robustness of the static solution procedure enables complete access to the multiplicity of solutions occurring immediately after the onset of bifurcation, as well as to the settled post-bifurcation states.

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Discrete Network Modelling of Topology-Property Relationships in Rubbery Networks

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Key Words: Rubber elasticity, Micromechanics, Constitutive modelling, Hydrogels, Elastomers

Understanding the relationships between network architecture and mechanical properties in crosslinked networks is critical for the design of soft materials such as elastomers and hydrogels. Yet, commonly-used constitutive theories of rubber elasticity (e.g. the 8-chain or the full-network models) rely on idealised network representations which ignore the role of network imperfections. Alternative representations have been proposed based on Bethe lattices in the context of linear elasticity (e.g. the Phantom model) but it is unclear how such approaches can be extended to large deformation. A new strategy is needed to explore structure-property relationships based on more realistic network repesentations, which could in turn inform the development of predictive constitutive theories.

In this contribution, we use computational random network simulations to investigate the elastic properties of hydrogels, building on our previous works [1, 2]. A new algorithm is proposed to generate random networks with controlled topology in terms of crosslink functionality, chain density, and chain end-to-end distance distribution. Several topological features are considered, including the degree of interpenetration of the chains, the presence of topological defects (dangling ends, loops), and polydispersity. The mechanical behaviour of random networks is simulated up to large deformations, and results are compared to available semi-analytical estimates and experimental data for tetra-PEG hydrogels [3]. Implications for the design of networks with improved properties are discussed.

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Effect of Molecular Structure on Mechanical Properties of Polycarbonate: A Coarse-grained Molecular Dynamics Study

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Key Words: Polymer, Simulation, Tensile strength, Radius of gyration, Entanglement

Polycarbonate finds a wide range of applications as structural materials and thus is drawing increasing attention in both scientific and industrial communities, owing to the prominent mechanical and physical properties. It is widely accepted that polymer mechanical properties are essentially related with the molecular structure [1]. In our previous coarse-grained molecular dynamics (CGMD) simulation for polycarbonate, the effect of molecular entanglement on maximum stress was investigated. As the number of entanglements was varied by altering the molecular weight [2], the causal effect of the number of entanglements on maximum stress remained unclear by confounding with the effect of molecular weight. This study therefore aims to reveal the effect of chain molecular entanglement and spatial distribution on fracture behavior as follows: The molecular entanglement, spatial distribution, and fracture behavior are quantitatively described by the average number of entanglements per monomer (N_e), root-mean-square of radius of gyration (R_g) and maximum stress ($\sigma_{\max}$), respectively. In this simulation, uniform weight polycarbonate structures with the systematical variation of N_e and R_g are generated by varying equilibrium temperature profiles and initial arrangements of molecules, respectively. Uniaxial tensile deformation is applied to each simulation cell at a constant strain rate, and the stress-strain relationships are obtained. We found significant effects of N_e and R_g on the maximum stress; for instance, the molecular structure of a higher radius of gyration leads to higher maximum stress with a constant molecular weight. Bivariate nonlinear regression analysis is performed to obtain description of maximum stress as a function of the radius of gyration normalized by molecular weight and the number of entanglements.

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Experimental and Numerical Study on Water-affected Adhesion of Polyacrylamide Hydrogels

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Key Words: *hydrogel, water content, physical adhesion, adhesion energy*

Hydrogels are widely used in flexible electronics and biomedical fields due to their superior stretchability and biocompatibility. Previous studies have demonstrated that the water content has significant effect on the elastic and fracture behaviours of hydrogels. However, the effect of water content on hydrogel adhesion has not been systematically explored. In our study, we first carry out a series of experiments on polyacrylamide hydrogels with a wide range of water content and find that the physical adhesion properties of polyacrylamide hydrogels are related to the water content. With the decreasing water content, the adhesion energy of polyacrylamide hydrogels undergoes four stages. The surface chain density, water molecules on the surface, bulk energy dissipation, and effective contact area of the polyacrylamide hydrogel are considered to synergistically contribute to these four stages. Specifically, at extremely low water content of about 30%, polyacrylamide hydrogels exhibit one order of magnitude higher adhesion energy than that at relatively high water content. It is also found that with the decrease of water content, the maximum peeling force presents a similar trend to that of the adhesion energy. To fully understand the effect of water content on hydrogel adhesion, a finite element method is further adopted to simulate the water-affected adhesion of the hydrogel attached to a rigid substrate, in which some parameters can be obtained from the experimental work. According to these discoveries, we can control the adhesion performance of a hydrogel by simply adjusting the water content, and even achieve reversible adhesion.

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Machine-learning Assisted Coarse-grained Molecular Dynamics Model Development of Double Network Hydrogels

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Key Words: *Double Network Hydrogels, Machine-learning, Coarse-grained Model, Molecular Dynamics*

Double network (DN) hydrogels are composed of two layers of crosslinked polymer networks. They have higher stretchability and greater toughness than regular hydrogels, making them promising applications in tissue engineering, drug delivery carriers, fluid actuators, and other fields. However, the experimental study of mechanical properties of DN hydrogels has some shortcomings, such as complex experimental process, high research cost, and low efficiency. Herein, coarse-grained molecular dynamics (CGMD) models of DN hydrogels are proposed by combining molecular dynamics (MD) simulation and machine learning (ML), to learn the relationship between crosslinked networks structure and their mechanical properties. The DN hydrogel CGMD model developed by ML simplifies the details of the all-atom model, reduces the degree of freedom of the simulation system, and saves the computational cost. The results obtained from the CGMD simulations are used as training data sets. The force field parameters are optimized by the artificial neural network. The results of this work provide general CGMD FF parameters and illustrate that it is possible to simulate large-scale complex hydrogels model models.

Mechanical Property Prediction of Single-Network Hydrogel Using Machine Learning Framework

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Key Words: *Machine learning, Hydrogel, Mechanical property, Predictive modeling*

Hydrogel has a complex network structure with inhomogeneous and random distribution of polymer chains. Much effort has been paid to fully understand the relationship between mesoscopic network structure and macroscopic mechanical properties of hydrogels. Recently, machine learning algorithms are becoming an important tool in the fields of mechanics of materials, attributed to its power to predict materials properties. In this study, we develop a machine learning framework to predict the mechanical properties of single-network hydrogel from polymer network structures. The constructed deep learning models are able to capture the nonlinear mapping from mesoscopic hydrogel network structural model to its macroscale mechanical property. The implemented machine learning framework provides a guidance to predict the nominal stress–stretch curves of hydrogels under uniaxial tension, and the framework also demonstrates the potential for predicting mechanical properties under more complex boundary conditions. Our results show that the end-to-end machine learning framework can effectively predict the mechanical properties of hydrogel within a wide variety of mesoscopic network structures, which demonstrates that the deep learning models are able to capture the internal relationship between complex network structures and mechanical properties. We hope this approach can provide guidance to structural design and material property design of different soft materials.

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Modelling the packing process of fiber/polymer composite powder in additive manufacturing

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Key Words: *Additive manufacturing; Discrete element method; Polymer; Glass fiber; Packing density; Surface roughness*

Fiber-reinforced polymer composites printed via additive manufacturing (AM) have gained great popularity because of their enormous potential for various applications in the automotive, aerospace, and biomedical industries. The main concerns on the AM of high-quality composite parts are the void content and fiber orientation, which are closely associated with the packing characteristics of powder beds. A discrete element model has been developed to study the packing quality of glass fiber/polyamide 12 composite powder in powder bed fusion AM. The geometric shapes of polymer powder particles and fibers are represented by multi-sphere particles and sphero-cylinders, respectively. The numerical model helps to understand the flow dynamics of composite powder particles and the formation mechanisms of voids in the powder packing process. The numerical model has been utilized to analyze the effects of packing parameters on the packing quality of the powder bed. The simulation results reveal that the increase of the powder layer thickness is beneficial to increasing the packing density and lowering the surface roughness of the powder bed. A high spreading velocity degrades the packing quality of the powder bed. A small number of fibers in the composite powder are in favor of the packing quality, while excessive fibers reduce the packing quality of the powder bed. The numerical simulation can serve to guide processing parameter optimization for improving the dimensional accuracy and minimizing the porosity in AM-printed parts.

Structural optimization design of intelligent hydrogel-based soft devices

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Key Words: *hydrogel-based soft device, topological optimization, moving morphable void and component, geometric nonlinearity, anisotropy*

A systematic approach is proposed to address the issue of shape and topology optimization of hydrogel structures involving recoverable large deformation in this paper. The thickness of the hydrogel layer and the fiber orientation of the fiber-reinforced hydrogel are taken as design variables in the shape optimization. The outline and material distribution of the hydrogel structures are described as the design variables by the explicit moving morphable voids and components in the topology optimization. In order to deal with the convergence issue of the intermediate process of nonlinear optimization, a material interpolation model is established and an adaptive mesh technique is used. Furthermore, the objective function is the displacement of specific nodes to ensure that the swollen structure achieves a unique actuation effect. The adjoint sensitivity is derived based on the mapped element density and the boundary evolution of the structure. Finally, several examples of optimization of isotropic and anisotropic hydrogel structures are used to prove the effectiveness and applicability of the proposed method. 4D printing experiments are also provided to demonstrate that the explicit topology obtained by this method can be directly used in the manufacture of hydrogel based soft devices.

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Study on Chemical Potential-Induced Shape Memory Behavior of Hydrogels

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Key Words: *Shape Memory Hydrogel, Constitutive Model, User-Subroutine*

Shape memory hydrogel (SMH) is a new type of the soft smart material, which can transfer from the temporary shape to initial shape when immersed in water. Different with the traditional shape memory polymer, the shape memory process of SMH is an adiabatic process, and the excellent deformability of the hydrogel allows us to pre-program more complex temporary shape. There is no constitutive model that can describe the shape memory behavior for hydrogels induced by chemical potential in an adiabatic process before. In this work, a constitutive model for SMH induced by chemical potential is established. In proposed model, we consider that the SMH consists of two phases, dense phase and sparse phase. The stored deformation is introduced in the dense phase to describe the shape memory effects (SME) of the SMH. The proposed model is further implemented in ABAQUS using the user-subroutine UMAT. We simulate SME of SMH under uniaxial loading, three-point bending, twisting. The comparison between the simulation and the proposed model for the SME of SMH under uniaxial loading shows good consistency. From the simulation for three-point bending and twisting loading cases, it can be demonstrated that the proposed model can describe the SME of SMH under complex and large deformation.

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A new efficient methodology for the analysis of mechanical metamaterials with elastic instabilities

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Key Words: Metamaterials, Reusable Energy Manipulation, Isotropic Microarchitectures

This work approaches the problem of the design of mechanical metamaterials including, as a distinguishing feature, instabilities in the elastic regime. Among the various opportunities offered by this characteristic [1], is the manipulation of the deformation energy. In this sense, metamaterials including elastic instabilities are known to exhibit reusable energy-trapping or energy-dissipation [2].

We present a novel methodology for the analysis of microarchitectures including instabilities. The strategy largely reduces the computational effort if compared with full models of non-linear volumetric finite elements or with non-linear beam elements. As a consequence, it allows to enlarge the analysis to more unit cells within the body of the metamaterial and to evaluate efficiently a greater number of topologies, proving to be especially suitable for use in processes of optimization of the microarchitecture.

Noting that existing designs of this class of materials only achieve energy manipulation in specific predifined loading direction, in this work, we center the design aim in obtaining reusable multidirectional isotropic energy manipulation with this technique. This is in accordance with a more realistic use of the metamaterials where general boundary condition do not establish a priori the loading direction.

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Computational Design of a Multiresonant Layered Acoustic Metamaterial for Low-Frequency Noise Attenuation

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Key Words: *Computational Material Design, Metamaterials, Low-frequency noise attenuation.*

For years, the concept of metamaterials has been used in the field of acoustics to refer to architected materials with the unnatural ability of attenuating sound in certain frequency bandgaps, thanks to local resonance phenomena. In this context, novel numerical tools under the Computational Material Design (CMD) umbrella, including multiscale frameworks, model-order reduction techniques, and topology optimization methods, have been combined to characterize such kinds of exotic behaviours enabling the design of optimal acoustic metamaterials with enhanced sound attenuating properties. In particular, a computational homogenization model is proposed, which is capable of capturing the effective macroscopic response triggered by local resonances in the metamaterial's microscale [1]. This numerical model has been successfully validated through an experimental sound transmission loss (STL) measurement of a 3D-printed acoustic metamaterial prototype [2].

As a next step in the computational design of acoustic metamaterials, the novel concept of Multiresonant Layered Acoustic Metamaterial (MLAM) is proposed as a potential solution to two major challenges still present in the acoustic metamaterials technology: (a) the narrowband nature of their attenuating capabilities, and (b) the complex manufacturing processes. The MLAM technology addresses the first issue by basing its design on coupled-resonances mechanisms that translate into a double-peak STL response (allowing to extend the attenuation bandwidth, even at low-frequency ranges). Furthermore, the layered-based structure makes the MLAM suitable for large scale manufacturing, for instance, through well-established lamination and die-cutting processes presently available in the industry [3]. In this regards, applying CMD tools to the MLAM design can potentially make the acoustic metamaterials technology feasible for the market.

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Modular-topology optimization arising from free material optimization and hierarchical clustering

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Key Words: Modular-topology optimization, Free material optimization, Wang tiling

Designing efficient modular structures and mechanisms demands solving two optimization task: optimizing the topology of individual modules and choosing their optimal placement in a product such that the modules synergistically cooperate. In our previous work on the minimum-compliance design of modular truss structures [1], we addressed this problem in a concurrent setup, combining a meta-heuristic method for updating the modular assembly plan with a second-order cone programming to generate the optimal truss-like topologies of the modules. Here, we present our recent results [2] on a computationally more efficient, bi-level sequential strategy applicable to continuum structures and mechanisms.

First, using the free material optimization, we determine the optimized distribution of stiffness tensors at the product scale. Next, we partition the stiffness tensors into a given number of clusters by a novel deterministic algorithm. Interpreting the outputs of the clustering algorithm within the Wang tiling formalism [3] yields the sought-for assembly plan. Finally, topology of individual modules is obtained from the standard, single-scale topology optimization based on the Solid Isotropic Material with Penalization interpolation scheme with the design space reduced by a mapping reflecting the modular assembly plan.

We illustrate the performance of our method on four two-dimensional problems: the modular minimum-compliance Messerschmitt-Bölkow-Blohm beam, two modular compliant mechanisms (an inverter and a gripper), and a combined modular design of both mechanisms, illustrating the reusability of the optimized modules. We demonstrate that by choosing the number of clusters we can compromise between a Periodic Unit Cell-based design of a material microstructure and a traditional full-scale topology optimization. Our method thus opens the way for the rational design of modular metamaterials and mechanisms at the material level.

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Multi-material topology optimization of microstructures using strength criteria

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Key Words: *Topology Optimization, Multi-Material, Stress, Microstructures, Homogenization*

Structural optimization plays an important role in the construction industry, leading to more material-efficient structures, promoting then the sustainability of this sector. One of the strategies to perform structural optimization is through Topology Optimization (TO). Single-Material Topology Optimization (SMTO) has been extensively studied over the past decades (see e.g., [1]). Regarding the Multi-Material Topology Optimization (MMTO), there is not that much work especially in microstructural design. MMTO is a current research topic, boosted by rapid developments in Multi-Material Additive Manufacturing (MMAM) (see e.g., [2]). It has been shown that multi-material design solutions, compared to single material, can lead to better performance (e.g., compliance and stress levels) [3-5].

This work addresses MMTO of a periodic composite material unit-cell considering two solid materials plus void, with properties predicted by homogenization, using strength and stiffness design criteria. Firstly, the compliance minimization with mass constraint MMTO problem is solved here. Then, one performs a stress-based MMTO problem where the maximal von Mises stress is locally minimized in the unit-cell. Two different types of design solutions are investigated in this latter case. On one hand, the two solids coexist being bonded together across sharp interfaces. On the other hand, a Functionally Graded Material (FGM) is obtained as an extensive smooth variation of material properties on account of varying composition's volume fractions of both solids throughout the design domain. From a computational cost viewpoint, performing the stress-based MMTO has two main bottlenecks: the stress sensitivity analysis and the optimizer runtime. Therefore, the stress derivatives are computed using the adjoint method in a parallel fashion, and the optimizer (MMA, see [6]) is here parallelized to speed-up its runtime when many constraints (say thousands of stress constraints) are considered.

The results show that multi-material designs can outperform single-material ones, both in stiffness and strength design criteria. More specifically, the obtained optimal designs of the compliance-based MMTO are stiffer and stronger than the single-material counterparts for the same mass requirement, on account of removing all void present in the microstructure. On the other hand, the stress-based MMTO designs for the same material volume show a decrease in the maximum stress on the microstructure on account of allowing an increased compliance. The FGM designs approximate fully stressed designs which excel in stress mitigation.

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Multimaterial Microstructural Design using Neural Networks

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Key Words: *Topology optimization, neural networks, multi-material, architected materials.*

Topology optimization is an effective design tool for generating novel, high-performance material architectures. In particular, multi-material microstructural designs have demonstrated superior properties [1,2]. In this work, we extend the neural-network-based representation, sensitivity analysis, and topology optimization proposed in [3] to design microstructures. The salient features of the proposed framework are: (1) the number of design variables is only weakly dependent on the number of materials considered, (2) it inherently guarantees that the partition of unity is satisfied, (3) it leads to a crisp and differentiable material interface, and (4) supports automatic sensitivity analysis for different objectives. We demonstrate the framework using numerical experiments and validate via physical testing of printed components.

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Multiscale Topology Optimization for the Design of Patient-Specific Orthotic Devices

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Key Words: Multiscale topology optimization, Metamaterials, Patient-specific application

New trends in additive manufacturing have been influencing the design phase of structures in order to unlock unexplored possibilities in terms of achieved geometries and performance. In this regard, several mathematical techniques have been proposed in the scientific and industrial community for the design of both macro- and micro-layouts, properly engineered for diverse objectives.

We present a two-step multiscale topology optimization framework for the design of innovative cellular materials at the microscale, and for the identification of optimized multi-material configurations at the macroscale. Firstly, we employ the microSIMPATY algorithm to devise a set of periodic reference cells that target desired physical goals and comply with given design constraints [1]. This ensemble is referred to as a dictionary of cells. As a second phase, we employ the newly-designed cells to topologically optimize the macroscopic structure, by identifying different regions of the domain where the cellular materials have to be alternated, in accordance with prescribed objectives and requirements [2].

After the formalization of the multiscale paradigm, the proposed algorithm is verified and validated for the design of patient-specific orthopedic insoles, by proposing innovative solutions that outperform standard approaches [3].

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A thermal strain energy calculation method of imperfect functionally graded sandwich cylindrical shells for wave propagation analysis

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Abstract

A theoretical investigation is developed to study the wave dispersion characteristics of imperfect functionally graded material (FGM) sandwich cylindrical shells composed of metal core and two functionally graded materials (FGMs) surface layers in the thermal environment. The temperature-dependent material properties are assumed to vary continuously along the thickness direction. Two types of porosity in FGMs layers of sandwich shells are considered. To describe the porosity effects, the porosity function composed of the porosity distribution function and porosity volume fraction is introduced. A novel thermal strain energy calculation method for cylindrical shell structures in high-temperature environments is developed. The Hamilton's principle is used to derive the wave motion equations, which govern the wave propagation behaviors. The analytical dispersion relations for the wave propagation of imperfect FGM sandwich shells in a thermal environment are obtained by solving a generalized eigenvalue problem. In addition, detailed studies are conducted to emphasize the parameter influences on wave propagation characteristics of imperfect FGM sandwich cylindrical shells.

Keywords: functionally graded sandwich structure; porosity; cylindrical shell; wave propagation; thermal stresses.

Computational Metamaterial Beam Modeling of Topological Phase Transition via Periodic Alternate Elastic Foundation

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Abstract

This study investigates the bending characteristics and topologically protected wave propagation of phononic crystal beam on periodic alternate linear elastic support. Timoshenko beam theory is employed to construct a computational model and derive the vibration governing equation. Subsequently by applying Bloch theory, the theoretical dispersion relation is calculated by transfer matrix method (TMM). The accuracy and reliability of TMM solutions are then verified by comparing with the finite element numerical results. Minor difference due to the assumption of Timoshenko beam theory is observed. A new method by tuning stiffness of elastic foundation is proposed in this study to break spatial symmetry and to tune the band structure. It is well acknowledged that a homogenous beam resting on elastic foundation exhibits a band crossing (BC) point and a bandgap which starts from 0 Hz. After breaking system symmetry by tuning elastic support in a periodic alternate manner, the BC point is broken and the other bandgap occurs. Furthermore, mode shape inversion can be observed and Zak phase transition can be calculated, which are essential for topological design purposes. Based on a unit cell analysis, we propose a supercell model by periodically arranging unit cells with the corresponding phase states and the topologically protected interface mode (TPIM) is analyzed. A parametric study of elastic foundation tuning parameter on TPIM frequency and quality factor is conducted. Finally, we design several sections or material defect conditions to demonstrate the defect- and disorder-immune properties of this beam-foundation system. The newly proposed topological phase transition generation mechanism can provide ideas and be extended to other mechanical and dynamic systems.

Keywords: elastic foundation; metamaterial; Timoshenko beam; transfer matrix; topological protected interface modes.

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Thermal metamaterial for heat manipulators

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Key Words: Thermal devices, Heat manipulators, Thermal metamaterials, Optimization, Isogeometric analysis (IGA)

Recent advances in material science and physics have sparked a renaissance in heat transfer research. Accordingly, the remedies to global issues such as global warming and the energy crisis also ask for advanced heat transfer devices, that can provide improved efficiency, accuracy, adaptiveness, tunability, and compactness compared to traditional heating, cooling, and harvesting energy. At the macroscale, heat manipulators are one such device that controls and manipulates the heat flow to achieve a specific objective (such as concentrating heat flux at a specific region, cloaking the obstruction in heat flow, etc.). The heat manipulators largely avail of the conductive thermal metamaterials due to their well-defined structure and unique properties [1, 2] that are not possible with naturally occurring materials. In a thermal metamaterial-based heat manipulator, the control on heat conduction is achieved by engineering the thermal conductivity, and consequently, the thermal design plays a pivotal role in its performance and reliability. The present work focuses on maximizing the efficiency of several heat manipulators with keeping manufacturing feasibility in consideration. In our work, we consider a thermal metamaterial composed of two materials as a heat manipulator. The effect of properties of member materials, their configuration, as well as incident flux on the objectives of the heat manipulators, is studied [1, 2, 3]. We also demonstrated a heat manipulator with dual objectives and its sensitivity to shapes, material properties of member materials, and dependency on each objective. Isogeometric analysis (IGA) (for solving the boundary value problem) and a gradient-free optimization algorithm are utilised.

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Vibration properties of functionalized diamane

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Key Words: *Diamane, Functional group, Vibration properties, Molecular dynamics simulation*

Low dimensional sp^3 carbon nanostructures have attracted increasing attention recently, due to their unique properties and appealing applications.[1-3] The single layer diamond - diamane, a two-dimensional (2D) form of diamond with a bilayer sp^3 carbon nanostructure, has been initially predicted in 2009,[4] while its experimental synthesis has only been reported in 2019.[5]

This work carries out a comprehensive study on the impacts from functional groups on the vibration properties of diamane targeting the ultra-sensitive sensing applications. Based on large scale molecular dynamics simulations, different functional types are investigated, such as the ethyl, methyl and phenyl groups. The results show that different functional types lead to different local bond reconfigurations, and introduce different impacts on the vibration properties of functionalized diamane. Furthermore, the content and distribution of functional groups are also studied to illustrate their influence on functionalized diamane's vibration properties.

Previous study has revealed that the diamane has excellent vibration properties, which are promising for the construction of ultrasensitive resonator-based sensors.[3] This work provides a comprehensive understanding of the influence from functional groups on the vibration properties of functionalized diamane, which should be beneficial to the tuning of ultrasensitive nano resonators.

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Phase change materials for thermoelectric micro-energy harvesting

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Key Words: Phase Change Materials, Thermoelectric Energy, Marangoni, Porous Media

Low-consumption electronics, such as wireless sensors, wearable electronics, or embedded devices, are employed to monitor industrial processes, environmental variables, health parameters, etc. Low-power sensors are placed in locations ranging from the human body to distant spacecraft. While batteries usually power them, applications involving remote locations, extreme conditions, or the of autonomous systems make batteries impractical. Among the different autonomous sources of power aimed at low-power sensors, thermoelectric energy emerges as one of the most reliable renewable energy sources.

Thermoelectric generators transform temperature gradients across them into electrical energy through the Seebeck effect. Efficient TEGs demand a significant temperature difference between the semiconductor junctions. This drawback limits their use to circumstances where a high thermal gradient is available. An emerging solution to mitigate the limitation of low efficiency is to employ a heat storage unit to generate sustained temperature gradients. In this way, temperature fluctuations in time are transformed into temperature gradients in space. Heat storage units based on latent heat, as the Phase Change Materials (PCM), are especially convenient because of their exceptional thermal energy density, and that part of the energy flowing into the PCMs is used to change their phase instead of homogenizing thermal gradients.

We show how increasing the heat transfer in the heat storage unit embedding the PCM in metallic foams multiplies the electric energy output an order of magnitude with respect to conventional designs of thermoelectric micro-energy harvesters [1]. These designs can power sensors for structural health monitoring in aircraft, monitoring in spacecraft, or harvest daily thermal fluctuations [2, 3]. Also, we present a new concept to strongly enhance the conversion of ambient thermal fluctuations into electric power using the dependence with the temperature of the surface tension of liquids (Marangoni effect) [4]. Since it is based on a fundamental principle, it can be used as a foundation for further improvements to optimize the output of thermoelectric devices to power low-consumption electronics.

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Multiscale Actuated Shells Structures

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Key Words: Multiscale optimisation, shell structures.

This abstract presents the development of multiscale optimisation methods for 2D shell like structures manufactured using 3D printing technologies, it builds on the groups activities in 3D multiscale optimisation [1]. A novel parameterisation of a slowly changing small-scale geometry is used to produce a range of responses, most notably coupling of in-plane and out of plane characteristics to allow complex behaviour to be arrived at via formal optimisation approaches enabled by adjoint sensitivities. The shell formulation used allows large structural response to be considered and the non-linear responses to be optimised via a grading of the small-scale geometry characteristics.

Four design variables are used to describe the small-scale geometry. This small-scale geometry populates the large-scale shell domain and is the same thickness of a the shell but varies gradually in the the in-plane direction. The characteristics of the small-scale geometry is determined through homogenisation theory [2] for the in-plane stress-strain (analogous to the A term in Classic Lamination Theory (CLT), bending-moment (D) and coupling between bending and in-plane behaviour (B). A fourth order polynomial is then fitted to each of the 18 unique terms of the A, B, D matrices as a function of the four design variables describing the small-scale. These equations are the constitutive equation which link the design variables to the local shell characteristics. The small-scale geometry parameterisation is such that the top and bottom surfaces of the geometry can have a varying in-plane auxetic behaviour, having an effective Poissons ratio (after homogenisation for application in the large-scale optimisation model) ranging from less than zero (auxetic) to around 0.3. By varying the top and bottom surfaces with a smooth variation through the shell thickness all three terms of the A, B, D matrices can be tailored. In addition to this coupling the stiffness can also be varied using the parameterisation method to change the magnitude of the terms.

The shell formulation used in the large-scale model allows non-linear, large deformations to be modelled and optimised for subject to different applied loads or displacements. Both the large and small-scale models apply the finite element method as implemented in FEniCS. Optimisation for the shell response uses sensitivities from the discrete adjoint method. The spatially varying parameters were then reconstructed and printed to produce optimised responses of the shells for a range of different problems (see https://youtu.be/4nbrgUubOKo for an example problem).

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Multiscale Topology Optimization: a Case for Pareto-Optimal Metamaterials

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Key Words: Multiscale Topology Optimization, Pareto Efficiency, Metamaterials, Surrogate modelling

In recent years, research towards multiscale topology optimization (MTO) has gained interest due to the rapid rise of additive manufacturing techniques. A recent trend in the field of MTO is the focus on families of metamaterials such as lattices with a parametrized unit cell [1]. Usually, these metamaterials are homogenized for varying parameters after which the interpolated homogenized properties are employed for optimization on the macroscale. In case the volume ratio is the only parameter, SIMP-like curves are obtained [2]. Although choosing a predefined microstructure family ensures connectivity and even improves numerical efficiency due to the reduced parameter space, the design optimality is inherently reduced. Indeed, any choice for a certain family of metamaterials restricts the design space, leading to sub-optimal designs.

Although ensuring connectivity and, more generally, manufacturability, is a necessary constraint, it is argued that optimality is often too severely restricted in recent literature. This talk proposes a novel way of looking at metamaterials, allowing for comparison based on their merits in a multiscale homogenization setting. Hereto, the principle of Pareto-optimality is employed by stating that the least a (meta-)material designer can do is ensuring its metamaterials are optimal 'in some homogenized sense'. More specifically, instead of restricting oneself to a family of metamaterials such as lattices with a cubic unit cell, one can and should instead choose the family of Pareto-optimal metamaterials: structures where one cannot improve an element of its homogenized stiffness tensor without jeopardizing either its weight or other stiffness tensor elements.

Such Pareto-optimal materials are then shown to lie on a Pareto frontier, a differentiable, high-dimensional manifold parametrized by the hyperparameters of a novel material design problem. Restricting the microstructural layout, e.g. by using a unit cell described by a low number of parameters, is shown to have severe consequences for the homogenized properties, effectively pushing the Pareto-manifold towards lower performance. Finally, a novel framework for MTO is proposed based on a surrogate model of the Pareto-optimal microstructure manifold. An implementation of this framework is provided and its advantages with respect to optimality, manufacturability and efficiency are highlighted.

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Two-Scale Topology Optimization respecting Buckling on Micro- and Macroscale

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Key Words: *Topology Optimization, Multiscale, Multiobjective, Buckling*

With the advances in additive manufacturing components with fine details gain more and more focus. The freedom of design allows for components with solid parts as well as finer substructures like lattices. Two-scale topology optimization, where the general topology is given on a macroscopic scale and finer details, like e.g. infill, are described on a microscopic scale, can help to design such components in an optimized sense with respect to some criteria. Though the use of lattice structures improves a component's compliance only under certain prerequisites, it seems to provide a large enhancement in terms of buckling stiffness of the whole component [1]. However, the introduction of fine details can lead to buckling of individual lattice cells.

In this presentation, we focus on a two-dimensional isotropic lattice structure built out of equilateral triangles, which, in an extruded version, is common as infill in additive manufacturing. To predict the buckling behavior on the level of the individual cells we use homogenization on a representative volume element (RVE), which encompasses more than one cell to also capture modes with a wave length greater than the cell size. We present a worst-case-model describing the cell buckling load factor on the macroscopic scale, which depends on the local porosity of the (possibly graded) lattice and the local stress. The model is developed taking into account uniaxial, biaxial and shear stresses. This enables us to use a scale-decoupled approach in the optimization of a component, which drastically reduces computational cost, but still respects buckling on both scales. We provide numerical results of simultaneous optimization of compliance and buckling on both micro- and macroscopic scale. We conclude with a validation of dehomogenized designs and a comparison of the predicted and actual cell buckling load factor.

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Controlling Failure Regimes of Brick-and-Mortar Structures through Shape

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Key Words: *Bioinspired, architected materials, nacre, micromechanical modelling, Cohesive Zone Model, Additive Manufacturing*

Natural materials, such as nacre, often exhibit exceptional combinations of properties, which is a result of the specific geometric arrangement of multiple materials across multiple length scales. One particular design motif that has been observed in nature is the Brick-and-Mortar structure, which is charaterised by stiff, discrete bricks in a staggered arrangement and a soft interfacial material between the bricks. Materials with this design motif commonly exhibit simultaneously high toughness and high strength, providing a motivation to replicate the motif synthetically. Synthetic replication of these structures has been made possible recently with the rise of multi-material additive manufacturing, which allows for high spatial control of multiple materials in a single part. To effectively utilize the synthetically manufactured Brick-and-Mortar structures for applications, a good understanding of the structure-property relationship, and underlying deformation mechanisms, is required.

In this work we present a finite-sized micromechanical-based analytical model to study the effect of the geometry of brick shapes on failure regimes of Brick-and-Mortar structures. The proposed model utilises the Cohesive Zone Model to capture the behaviour of the soft phase. It will be shown that such composite structures exhibit 'two-peak' and 'peak-plateau-peak' failure, differing in their ability to distribute damage through the normal layers prior to failure. Furthermore, we demonstrate that these failure regimes can be controlled by varying the angle of the shear layer with respect to the normal layer. We further extend the modelling of the Brick-and-Mortar structure to FEA, utilizing the Cohesive Zone Model, to better predict the composite properties, as well as to extend our prediction of failure regimes to 3D shapes. The prediction of trends in the failure regimes, and the corresponding composite properties, are validated with experiments using Additive Manufactured Brick-and-Mortar structures.

Deep Learning Model to Predict and Generate New Protein with Desired Secondary Structure Content

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Keywords: *Deep Learning, protein structure, secondary structure, structural proteins, artificial intelligence, materiomics*

Abstract: The diversity of protein function depends on a local structure derived from the primary amino acid sequence. Structural proteins are the foundation of many biomaterials and is also key constructors and functional components of all life. As the function of protein is determined by its folding structure of a tertiary structure, we try to control the secondary structure content to design the functional protein we want. The primary structure will affect the secondary structure and then affect its tertiary structure. However, it's difficult to design its tertiary structure directly. Here, we provide a deep learning model not only can predict the secondary structure content of the protein from the primary sequence, but also can rearrange the amino acid sequence in the primary structure of the protein to generate a new protein structure with the desired secondary structure content. The secondary structure content of the protein is essential to design a target material function, especially the protein of mechanical properties. Alpha helix and beta sheet are the two most common secondary structures, we use convolution and circulating architecture and natural language models, which can predict the contents of these two basic types of secondary structures, and through the genetics algorithm model rearrange the amino acid sequence in the protein primary structure to generate a new protein structure having the desired secondary structure content. The alpha helix and beta sheet content predictions show excellent agreement with training data and newly deposited protein structures that were recently identified and which were not included in the original training set, and we also generate new primary structure of protein with target secondary structure content successfully. Our model can be widely used in the development of any drugs, vaccines, proteins and other biological material, and be applied to material design and development and other biomedical industries.

Design, Modeling, and Manufacturing of Nature-Inspired Architected Materials Through Unsupervised Deep Learning

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Key Words: *Machine Learning, GAN, Bioinspired, Architected Materials*

The design of materials inspired by nature is an emergent topic of great interest, pushing the envelope to create a variety of new material platforms for sustainable technologies. This is motivated by the nature-inspired design paradigm: nature has succeeded in creating strong and tough materials out of weaker organic or ceramic building blocks by architecting them at multiple scales, and as such, innovation can be accelerated by harnessing nature's design principles through biomimicry and beyond, exploiting these principles in novel designs further optimized for human and societal needs[1]. Here we report the development of a deep learning-based approach using a manipulable GAN model[2,3] that enables the generation of de novo 2D and 3D material structures with an inverse tomography approach. The GAN model is used to generate, through movements in latent space, continuous slices of images that are tiled into engineered quasi-2D materials, or reconstructed into 3D geometries that can be further modeled and manufactured using 3D printing. Not only can the concept be used to construct novel materials that mimic natural designs, it also allows for a transfer of information across manifestations, using the latent space as the mediator. This enables us to use information from disparate sources to be translated into material designs. We illustrate the concept here for new materials inspired by leaf microstructures, showing how biological 2D structures can be used to develop novel architected materials in 2 and 3 dimensions. With further refinement and engineering, this work opens new avenues for nature-inspired materials beyond the traditional inspiration or mimicking of natural systems.

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Extremely deformable materials inspired by cytoskeletal networks

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Key Words: *Multiscale modeling, Bioinspired design, Extreme material deformability, Intermediate filament networks, Cytoskeletal mechanics*

Material applications involving large cyclic deformations are ubiquitous, ranging from consumer's goods to soft actuators and novel biomedical devices. Epithelial monolayers – cohesive cellular sheets commonly attached to a matrix and lining free surfaces – face similar challenges. The need to repeatedly withstand large deformations has led evolution to refine the structural arrangement of key cytoskeletal components (actin, microtubules, and intermediate filaments (IFs)) and hierarchical motifs (*e.g.* coiled-coils). Recent work highlighted that actin dilution in superstretched cells is accompanied by massive rearrangement of the IF network, whose entangled filaments eventually form a central knot and thick radial bundles that allow cell sheets to cope with extreme deformations [1, 2]. These multiscale characteristics, whereby the structural components may selectively yield, reorganize, and eventually recover, are reminiscent of recently-developed soft materials with unprecedented deformability, toughness, fatigue threshold, and low hysteresis [3, 4].

Inspired by this fascinating parallel between a technical and biophysical problem, we address the design of extremely deformable materials using concepts from epithelial IF networks. Borrowing from mechanics, geometry, and topology, we reverse-engineer the multiscale organization of entangled IF networks and define the conditions that lead to the formation of a stable central knot, enabling load bearing. Our analysis yields a rational link between the emerging material response under cyclic loading and the number, length, constitutive behavior, and degree of entanglement of IF bundles. Ultimately, we propose bioinspired design principles that allow tuning the macroscopic behavior of extremely deformable materials in view of specific applications requirements.

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Hierarchical bioinspired architected materials and structures

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Key Words: *Bioinspired, Lattice, Hierarchy, Topology, 3D printing, Additive manufacturing*

Nature is a stunning example of how–through the design and self-assembly of heterogeneous hierarchical structures–it is possible to combine and amplify the properties of the constituent building blocks of biological materials and optimize such materials for the environment in which they must survive. As evolution continues to drive the adaptive process of making natural materials over time, engineering is now attempting to emulate this extraordinary capability, lately via lattice materials and 3D printing techniques. Indeed, it is well known that, through the combination of optimized cellular architectures, high-performance lightweight materials with optimal combinations of high strength-to-weight and stiffness-to-weight ratios can be fabricated. However, the realization of such complex hierarchical structures with a micro- to macro-scale precision is still a challenge that can only be overcome with state-of-the-art additive manufacturing techniques. Despite the new widespread interest in lattice and hierarchical structures and the recent progress in the field of these materials, many concerns remain regarding their structural integrity due to the lack of well-structured guidelines for their design and a property database to assist in this process. The present research, therefore, aims to fill a portion of this knowledge gap through understanding how the effects of topology, hierarchical organization, and material distribution affect the mechanical properties of a simple design domain, here used as a case study. To this end, we adopt a comprehensive approach that combines computational mechanics approaches with additive manufacturing routes. We consider a beam subjected to four-point bending as a meso-structure. We select two unit cells with contrasting behavior, a bending dominated (single cubic) and a stretching dominated (face-centered cubic), and devise four different designs by introducing these unit cells within the design space. The various designs are created via a modular reconstruction with the ANSYS Mechanical APDL finite element software. The struts of the unitary cells are discretized with beam type finite elements and, through linear analysis, the relationship between structure and stiffness/weight ratio is analyzed. The outcome of this study allows us the probe the effect of the hierarchy, the effect of topology, relative density, and slenderness ratio (SR) of the strut on the overall mechanical behavior of the beam. In particular, we notice how the introduction different hierarchical levels may not be beneficial; this is even more evident when stretching dominated structures are involved. Instead, in the case of bending dominated structure the numerical study shows how the addition of further hierarchical levels can increase the stiffness performances, for low values of SR.

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How to protect a weak spot inside a load-bearing architectured material: a lesson from bone

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Key Words: *Bone, Cement Line, Damage Propagation, Architectured Materials*

Economic and environmental constraints are triggering the development of materials with enhanced mechanical efficiency and reduced over-dimensioning. These challenges can be met with so-called architectured materials, which have well controlled structural features sitting at intermediate length scales between overall component size and microstructure. However, architectured materials often contain potentially weak spots such as pores and interfaces, which can trigger damage. To minimize and predict failure in these materials, it can be instructive to consider how nature has coped with such problems. As an example, bone is a biological material that not only tries to minimize failure, but can also tolerate and repair damage. One essential feature enabling bone renewal is the presence of an intricate multiscale porosity to house blood vessels and cells. As a consequence, bone must avoid that stress concentrations around pores cause failure. Moreover, cracks forming due to daily loading must not reach the functional pores. In cortical bone, blood vessels are accommodated in the central canals of osteons, which are cylindrical features consisting of several concentric layers of bone lamellae and bordered by a thin protective sheet, called cement line. Osteons are important for bone toughness as incoming cracks can be deflected by the cement line or twisted by the lamellae. In our study, we combine computational modeling with 3D printing to explore the mechanical behavior of osteon-inspired materials. In analogy with the cement line in bone, the protective role of interlayers around a weak region is characterized using damage-based finite element analysis, which assumes that a critical equivalent plastic strain is needed to initiate damage and that damage evolution is controlled by a specific energy [1]. Increasing damage decreases stiffness and strength. We designed 2D notched models featuring a homogeneous matrix with a central hole, bordered by a thin interlayer. We systematically varied the position of the notch with respect to the hole as well as interlayer stiffness, yield stress and fracture energy. After finding the critical notch position that causes a crack to reach the hole, we introduced the interlayer around the hole and we investigated damage behavior. Our results indicate that even a minimal interlayer (having a thickness one order of magnitude smaller than the diameter of the hole) can have a large and non-trivial impact on damage mechanisms, influencing the interaction between the crack and the hole. Interlayers with yield stress smaller than matrix strength are able to trap damage, thus shielding the weak spot. Interlayers more compliant than the matrix can hamper the propagation of cracks after reaching the hole. We used 3D polyjet printing to prototype selected models with interlayers (cement line) printed using different material (stronger or weaker) than the matrix. Our prototypes showed a programmable failure behavior dependent on interlayer properties. This work demonstrates that bone's design strategy to hamper damage can be translated to higher length scales, even using completely different building blocks, into 3D-printed synthetic materials.

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Initial Yield Surface of Cellular Sheet TPMS Lattices

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Keywords: *Lode; TPMS; Metamaterials; Yield Surface.*

Due to the advancements in additive manufacturing and increased applications of additive manufactured structures, it is essential to fully understand both the elastic and plastic behavior of bio-inspired cellular materials, which include the mathematically-driven sheet/shell lattices based on triply periodic minimal surface (TPMS) that have received significant attention recently. The compressive elastic and plastic behaviors have been well established for many TPMS latticed structures, but not under multiaxial loading. Furthermore, TPMS lattices are computationally expensive to model explicitly (i.e., micromechanical) when used in latticing various structures for enhanced multi-functionality, and hence the need to develop an accurate yield surface function or criterion in order to model their plastic behavior in a homogenized approach. The majority of previous yield surfaces developed for cellular materials were developed for cellular foams [1, 2], and very few attempts has been made to develop a yield surface based on cellular lattices [3]. Furthermore, some of the few studies [4] that used the yield surfaces developed for foams to predict the yielding of cellular lattices, have found that such yield surfaces do not predict well the yielding of lattice structures under various multiaxial loading conditions. In this study, an initial yield surface is developed for sheet TPMS cellular lattices, which to our-best knowledge has never been attempted before, and is compared to the major yield surfaces that have been developed for cellular materials. The effect of different loading conditions on the effective yield strength of IWP sheet-based (IWP-S) TPMS lattice is numerically investigated. The simulations are based on a single unit cell of IWP-S under periodic boundary conditions, assuming an elastic-perfectly plastic behavior of the base material, for relative densities ($\bar{\rho}$) ranging from 7% to 28%. In order to account for the different loading conditions, the Lode parameter (L) is used [5]. The effect of L is studied over a range of mean stress values (σ_m) to understand the effect of both L and σ_m on the effective yield strength. In the plane of the von Mises equivalent stress σ_{VM} versus σ_m, σ_{VM} is maximum at $\sigma_m = 0$ and reduces in a parabolic and nearly symmetric manner with $\pm\sigma_m$ values. On the other hand, in the plane of σ_{VM} versus L, σ_{VM} is minimum at $L = 0$ and increases in a parabolic and nearly symmetric manner with $\pm L$ values. Using these relationships, the effective yield surface for IWP-S is characterized by σ_{VM}, the mean stress σ_m, L and $\bar{\rho}$. In the 3D space of the principal stresses, this yield surface is best described as a cocoa pod. The current developed framework can be adapted for generating yield surfaces for other lattice topologies.

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Multi-scale non-linear modeling of biomimetic composites using a coarse-graining approach

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Key Words: *Multi-material 3D printing, Bitmap 3D printing, Bioinspired design, Homogenization.*

Across time, Natural materials have adapted to their environments by developing a wide arrange of features (*e.g.,* functional gradients, multi-hierarchical organization) [1]. Today, voxel-based or bitmap additive manufacturing (AM, =3D printing) [2] allows incorporating such natural design paradigms into biomimetic composites with complex microarchitectures [3]. This technology uses stacks of binary images to define a composite, where each white or black pixel represents either 'hard' or 'soft' material deposition. However, large voxel counts and complex features make modeling the mechanics of such biomimetic structures extremely challenging and time-consuming. Here, we propose a novel coarse-graining approach based on non-linear foam-based constitutive equations [4] to facilitate the computational modeling of complex biomimetic composites at coarser length scales while maintaining the mechanical response of the composite at high resolution.

To determine the coefficients of the constitutive equations, we used data obtained from standard tensile tests of various composites with different hard material volume fractions (ρ). We additively manufactured these specimens using polyjet 3D printing techniques (Stratasys, USA) and tested them under tensile loading conditions while recording their deformations using digital image correlation. We used non-linear regression fit on the stress *vs.* strain data to determine the parameters of the foam-based constitutive equations. This process enabled us to predict the response of composites within the entire non-linear design space as a function of ρ. We used non-linear finite element code (Abaqus v.6.14) to perform numerical validations of these tensile tests.

Furthermore, we assessed and validated the performance of our coarse-graining approach by comparing our computational models with those of crack (mode I) experiments on biomimetic designs. These tests validated that this coarse-graining approach retains adequate mechanical response of a bitmap design while reducing computation times, even when complex features are present. Thus, the proposed approach offers a rapid, accurate, and reliable tool for designing, modeling, and optimizing advanced engineered biomimetic materials with tailor-made properties.

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Music-based proteins: new design opportunities for architected biomaterials

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Key Words: *Biomaterials, sonification, protein folding, molecular dynamics*

Biomaterials, especially proteins, bear many striking similarities to music that can be observed in how both exhibit long-range patterns and hierarchical constructions across time and length scales. They are both increasingly intricate yet neatly ordered networks built from smaller individual units, and thus, music can present a radical paradigm for further understanding the complexities of these biomaterials. Such relationships between music and biomaterials have been previously demonstrated in the sonification of existing proteins and the creation of an amino acid 'scale' via the ranking of vibrational modes. In this study, we present an algorithmic method for translating classical music, specifically excerpts of Leonard Bernstein's "Chichester Psalms", to de novo protein sequences to further elucidate the potential for existing composed musical language as a basis for biomaterial design. This case study also provides a pilot investigation into the capabilities of various predictive protein folding methods like trRosetta and the newly introduced AlphaFold2 for folding de novo sequences with no existing native counterparts. Moreover, the 3D predicted models provide the basis for an iterative generation of new sequences as well as an opportunity to create new musical compositions based on folding patterns and protein contacts. We further analyze the resulting protein structure models and sequences through MD simulation and comprehensive taxonomic profiles of the sequences made using BLAST reveal numerous sequence similarities to native bacterial and eukaryotic organisms. This endeavor demonstrates how understanding proteins within the framework of musical form and language opens doors to a holistic and revolutionary approach to functional biomaterial design.

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A high-precision partition coupled Eulerian-Lagrangian method for compressible fluid with large deformation

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Key Words: *Coupled Eulerian-Lagrangian method, Interface capturing, Compressible fluid, Partition weighted bidirectional mapping*

In the past few decades, numerical methods of solving hyperbolic conservation equations can be divided into Lagrangian and Eulerian methods. The Eulerian method is suitable for simulating fluid flow with large deformation, but often smoothed out discontinuities too much due to the limited number of grids. The Lagrangian method can avoid the numerical dissipation caused by the convection term, but the grid will be distorted and cause large errors. Although both Lagrangian method and Eulerian method have their own unavoidable difficulties, they can be combined in a certain way to give full play to their respective advantages.

A partition coupled Eulerian-Lagrangian method (referred to as PCELM) is applied to accurately track the interface and the contact discontinuity of the compressible fluid with large deformation. This method arranges splittable Lagrangian particles on the Eulerian grid to automatically track the discontinuous points, and adopts the partition weighted bidirectional mapping between the particles and the grids by using cubic interpolation function, which maintain the steep discontinuous transition in the discontinuous area. The partition weighted bidirectional mapping method weights the shape function by the coincident volume fraction of the particle domain and the grid domain, to improve the mapping accuracy and eliminate the oscillation across the grid. The PCELM avoids the the grid distortion problem of Lagrangian method, and makes up for the defect that the Eulerian method cannot accurately track the interface, so that it can accurately capture the contact discontinuity and the free interface.

Then the virtual particle method is introduced to solve the discontinuity of particles at the flow boundary, and to realize the inflow and outflow of particles and maintain the interpolation accuracy of the boundary. Aiming at the numerical fracture problem, the particle splitting method is developed to deal with the violent stretching of the particle.

Finally, a number of numerical tests are used to demonstrate the advantages of PCELM in capturing interfaces and discontinuities. The accuracy test shows that the CELM has fourth-order convergence accuracy, and the norm error of it is lower than that of WENO3 and WENO5 at lower grid numbers. Compared with WNEO3 and WNEO5, SOD and Woodward-Colella test shows that CELM can accurately tracks the shock wave and discontinuity by particles, and the value on the discontinuity is closer to the precise solution and the reference solution, and has lower dissipation. The dam break problem shows small gap between results of PCELM and experimental results, which reflects the advantage of particles tracking the free interface. The two-dimensional Riemann tests reflects shock wave resolution of different schemes. Also compared with WENO3 and WENO5, PCELM can obviously simulate the fine structure of the shock wave at a lower grid number, which reflects its low dissipation characteristics and the advantages of high-precision shock wave capture.

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Agglomeration Regimes of Particles in Shear Flow

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Key Words: *Particle Agglomeration, Smoothed Particle Hydrodynamics, Discrete Element Method, Dewatering*

Summary: In the mining industry, particle aggregation phenomena in solid-liquid separation are beneficial to accelerate slurry dewatering and improve the performance of thickening and filtration operations. The structural characterization of solid particle agglomeration is an essential part of optimizing the design of dewatering systems and can be investigated using particle-scale simulation. An atlas of different structural shapes of solid particle aggregates under different Reynolds numbers and inter-particle pair potentials can be generated based on the assumption that the solid-solid particle interaction is described by a given Lennard-Jones potential [1]. However, this assumption cannot accurately reflect the contact and adhesion behavior of solid particles.

In our computational simulation tool, a more accurate contact adhesion model was adopted to represent the interaction of solid particles by using Discrete Element Method (DEM). The fluid is modeled with Smoothed Particle Hydrodynamics (SPH). A combined SPH-DEM model is proposed here to model particle agglomeration in shear flow. The system is governed by three fundamental dimensionless groups: the Reynolds number *Re*, which measures the effect of the hydrodynamics; the Adhesion number *Ad*, which measures the 'stickiness' of the particles; and the solid fraction α, which measures the concentration of particles. Based on these three dimensionless groups, several agglomeration regimes are found in Figure 1. Within these regimes, the aggregates can have different sizes and shapes that go from long thread-like structures to compact spheroids. The effect of the particle-particle agglomeration model (Johnson–Kendall–Roberts or Derjaguin–Muller–Toporov) is also investigated. Once *Re*, *Ad* and α are known, the results are combined into 'agglomeration maps', which allow for a quick determination of the agglomerate type.

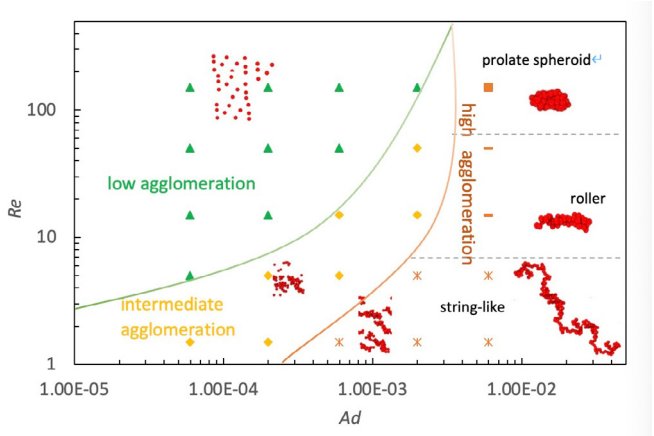

Figure 1: Agglomeration regime map. Illustrating the observed cases as a function of Reynolds and adhesion numbers at a solid particle volume fraction 4.2%.

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Development of Efficient and Accurate Simulation Method for Chemical Conversion Treatment Phenomena

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Key Words: Chemical Conversion Treatment, Etching, Solid Fluid Interface, Finite Differential Method

The chemical conversion treatment is a method for preventing rust and corrosion by a film precipitation reaction induced by an etching reaction on a metal surface, and is used for surface treatment of automobiles. Examples of the chemical conversion treatment include zinc phosphate treatment and zirconium chemical conversion treatment. Application of numerical simulations to the development of chemical conversion treatment agents is useful for understanding of the mechanism of the phenomenon and shortening of development time. On the other hand, in the chemical conversion treatment, the reaction is concentrated in the very thin boundary layer on the surface of the material and a steep concentration gradient is formed at the initial stage of the reaction. The naive application of the conventional method leads problems of error and increase in calculation time. In this study, we have developed an efficient and accurate finite differential method for chemical conversion processing. That is, we proposed a method to improve the analysis accuracy of the inlet, metal surface, and the region of the initial state where the reaction is intense by converting the spatiotemporal variable in the numerical analysis of chemical conversion treatment into an exponential function. In order to verify the effectiveness of the proposed method, the etching phenomenon of the steel sheet with an acidic solution was analyzed.

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Numerical modelling of the dissolution of composite particles

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Key Words: *Discrete Multiphysics, Dissolution Problem, Mass Transfer, core-shell microparticles*

Summary: We present the dissolution of composite particles utilising the Discrete Multiphysics [1] (DMP), a numerical model that combines particle-based techniques. We have focused on core-shell particles that have numerous applications in food-processing and healthcare industries. Figure 1 represents the time evolution of the dissolution of a single core-shell particle in fluid flow. It will be shown that DMP is a suitable tool for modelling the dissolution process due to its Lagrangian particle-based nature and can be utilised for modelling more complex structures.

The numerical results will be validated against available analytical and numerical data in literature through different mass transfer processes. We will conduct a systematic study on the dissolution of core-shell solute particles by considering the effect of fluid inertia and the ratio between the diffusion coefficient of core and shell materials. Thus, we will investigate the variations of Reynolds number and the Schmidt number ratio, respectively. We will conclude the discussion by providing design guidelines for specific applications of core-shell microparticles.

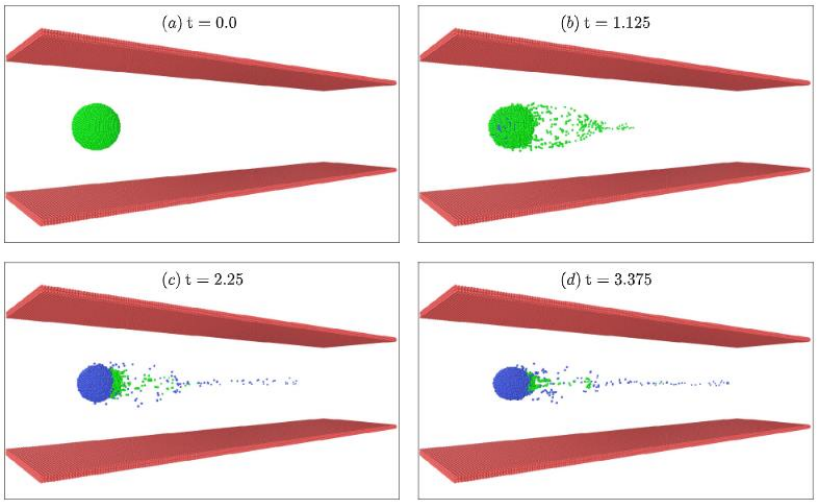

Figure 1: Dissolution of a core-shell particle at different simulation times; shell and core phases are shown by green and blue particles, respectively, while fluid particles are removed for better illustration.

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A low-cost resolvent analysis of flow around a bluff body

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Key Words: Resolvent analysis, Cylinder wake, Randomized method

In order to solve various environmental problems discussed around the world, it is of great importance to develop practical flow control methods for suppression of the vortex shedding in flow around a bluff body. However, assessment using the high fidelity numerical simulation such as direct numerical simulation requires an enormous computational cost to capture the turbulent phenomena accurately. To overcome this problem, McKeon and Sharma (2010) proposed the resolvent analysis, which is one of the modal analysis methods. So far, application of the resolvent analysis has mostly limited to one-dimensional flow, e.g., fully developed channel and pipe flows. Therefore, in the present study, we extend the resolvent analysis to a two-dimensional flow, i.e., flow around a circular cylinder. However, in two-dimensional flows, we need to solve the governing equations in the two-dimensional domain, so that the size of the matrix in the resolvent operator is drastically increased and the computational resource required becomes large. To reduce the computational cost, we develop a resolvent analysis based on the energy-conservative finite difference method on a staggered grid system. In addition, to reduce the matrix size, the randomized method proposed by Riberio et al. (2020) is applied. It is found that the present staggered grid-based randomized resolvent analysis is able to accurately compute the forcing and response modes as well as their singular values as far as a sufficient size of randomized sketch is used. Moreover, using this low-cost method, we analyze the forcing and response modes in the flow around a cylinder in detail. In the presentation, we will also propose effective flow control methods to suppress vortex shedding.

We thank Mr. Hikaru Murakami (Keio Univ.) for providing the DNS data and Ms. Riko Uekusa (Keio Univ.) for fruitful discussion. We also thank Dr. Kunihiko Taira and Dr. Jean Helder Marques Riberio (UCLA) for the instruction on the randomized resolvent analysis. This work was supported from the Japan Society for the Promotion of Science (21H05007).

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A one-way coupled Lagrangian-Eulerian procedure for the solution of landslide-generated waves

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Key Words: *Free-surface flows, Particle finite element method, Finite element method, Fluid dynamics, Shallow water*

This work presents a partitioned method for landslide-generated wave events. The proposed strategy combines a Lagrangian Navier Stokes multi-fluid solver with an Eulerian method based on Boussinesq shallow-water equations.

The Lagrangian solver uses the Particle Finite Element Method [1, 2] to model the landslide runout, its impact against the water body and the consequent wave generation. The results of this fully-resolved analysis are stored at selected interfaces and then used as the input of the shallow water solver [3,4] to model the far-field wave propagation.

This one-way coupling scheme reduces drastically the computational cost of the analyses while maintaining high accuracy in reproducing the key phenomena of the cascading natural hazard.

Several numerical examples are presented to show the accuracy and robustness of the proposed coupling strategy and its applicability to large-scale landslide-generated wave events. The validation of the proposed method is performed versus available results of other numerical methods, analytical solutions and experimental measures.

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Deep Learning-based Unsteady Flow Estimation: Nonlinear Convolution of Wakes behind an Oscillating Cylinder

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Key Words: Convolutional neural network, Machine Learning, State estimation, Unsteady flow

In our daily lives, there are many vibrating objects with fluid flows, e.g., flapping wings of birds [1], heat exchanger [2], and tidal power generator [3]. The detailed information about such flows can be utilized for flow control or anomaly detection via fluid flows; however, few available sensors in the practical situation make it difficult to obtain the flow information over the entire region. To tackle this issue, we here utilize machine learning. Machine learning has been regarded as an effective tool for fluid flow analysis thanks to its ability to consider nonlinearity. We estimate the flow field with an oscillating cylinder at the Reynolds number $Re = 150$ utilizing convolutional neural network (CNN) [4]. The CNN estimates the wake behind the cylinder from the flow field around it. The training data is prepared by direct numerical simulation (DNS). We prepare various types of datasets whose direction and frequency of vibration differ from each other. The present CNN model successfully estimates the flow fields, which are in qualitatively agreement with the reference DNS under any vibration condition. The L_2 error norm also suggests reasonable estimation performance, although it has a high dependency on the frequency. To clarify the cause of this, the cosine similarity is introduced as a measure of correlation between the snapshots. The evaluation using the cosine similarity reveals that the L_2 error norm tends to be smaller when the flow field has periodicity. This result indicates that we can achieve efficient training by reducing the number of snapshots according to the periodicity.

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Direct Numerical Simulation of Turbulent Flow Controlled by Wall Oscillation in Concentric Annular Pipe

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Key Words: *Turbulent flow, Annular pipe Flow, Wall Oscillation Control, Direct Numerical Simulation*

Drag induced by flow usually consists of contributions from pressure and skin friction, referred to as pressure drag, and friction drag, respectively. The friction drag accounts for about 50% of the total drag for an aircraft and about 100% of the drag for a pipeline [1]. Therefore, control techniques to reduce the skin-friction drag are essential in engineering from the viewpoint to improve energy efficiency in several decades. The wall oscillation technique is well known to reduce the skin-friction drag in the turbulent channel flow, e.g. [2]. In the present study, we employ the wall oscillation control technique and aim to investigate the skin-friction reduction effect of the turbulent flow in the concentric annular pipe using direct numerical simulations. The concentric annular pipe is widely used in fluid engineering. We expected to reduce the skin-friction drag efficiently by using the different radius of the inner and outer cylinders.

We apply the wall oscillation control for the inner and outer cylinder, and the control parameters are the amplitude A and the frequency f. We refer to the same control for the turbulent channel flow [3] to determine the range of the parameters. As a result, if the oscillations on both cylinders are synchronized, the maximum skin-friction drag reduction rate was 47% and 52 % at the inner and outer cylinder surfaces, respectively. On the other hand, if the oscillation is applied on the inner cylinder and the outer cylinder is immobile, the maximum drag reduction rate is 39% at the inner cylinder surface and decreases as the frequency increases.

In the presentation, we will discuss in detail, e.g., the drag reduction mechanism, the influence of the ratio between the inner and outer radius onto the control effect.

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DNS-CNN Simulation of Viscoelastic Turbulent Flow using U-Net

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Key Words: *Viscoelastic fluid, Turbulence, Deep learning, Surrogate model*

Viscoelastic fluid is a non-Newtonian fluid obtained by adding a polymer or surfactant to water. The characteristic feature of this fluid is the drag reduction due to the suppression of vortices by the intensification of polymer extension in turbulent flow conditions. This drag-reducing effect saves pumping energy in fluid transports. From the viewpoint of engineering applications, many experiments and numerical simulations have been carried out, but the flow mechanisms of viscoelastic fluids are still not fully understood. Numerical instability is one of the factors that hinder numerical studies. In numerical simulations of viscoelastic fluids, a constitutive equation is required as a governing equation, which should include viscoelastic stresses. However, due to the absent of a diffusion term in the constitutive equation, e.g., the Giesekus model, the numerical instability often becomes a problem at high Weissenberg numbers [1].

Deep learning has been widely used in the field of fluid mechanics with the aid of the recent development in computational hardware and the emergence of many network models. In fact, attempts have been made to address many issues in fluid mechanics, such as low-dimensional modeling, experimental-data processing, shape optimization, turbulence closure modelling, and flow controls [2]. Since the deep learning builds models from data, it is possible to discover essential features. Applying the model built by deep learning to the constitutive equation has a potential to extract features of viscoelastic-fluid turbulence and to solve the problem of numerical instability at high Weissenberg numbers.

In this study, we applied deep learning to construct a surrogate model of the constitutive equation to simulate the viscoelastic turbulent channel flow. We adopted U-Net, a convolutional neural network (CNN), to predict the conformation stress field from the velocity field obtained from direct numerical simulations (DNS). Using the trained U-Net, we demonstrated an integrated calculation of DNS and CNN in which the constitutive equations were replaced by the U-Net. The mean profile of c_{xx} (the streamwise normal component of the conformation tensor) and the flow field were reproduced with high accuracy by using U-Net. However, the prediction accuracy of c_{yy} (the wall-normal component) in the buffer layer, where polymer rotation is induced by vortices, is rather low. The predicted instantaneous field exhibit somewhat noisy distribution caused by the convolution operation in the U-Net. In the surrogate model of U-Net, we compared the result of the DNS-CNN simulation to the pure DNS. The obtained statistics showed a good agreement between both simulations.

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Evaluation of Drag Reduction Effect and Surface Stress on Riblet in Turbulent Channel Flow Using Direct Numerical Simulation

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Key Words: *Direct Numerical Simulation, Drag Reduction, Riblet, Stress Field*

A riblet is an object with a fine groove structure that can reduce the frictional drag of wall-bounded turbulent flows. For example, Sasamori *et al.* (2014) confirmed 12% drag reduction by a sinusoidal riblet in a turbulent channel flow [1]. Because of such a micro-groove structure, riblets poses a durability problem for practical use. Therefore, we focused on the force acting on riblets. Direct numerical simulation (DNS) of a turbulent channel flow was conducted with riblets generated by an immersed boundary method. Each riblet has rectangular cross sections with variable height and spanwise position changing by random Fourier series in the streamwise direction.

It is found through a flow visualization that when vortices are close to a riblet, the surface stress of the riblet is far from the mean wall shear stress without the riblets. This indicates that the approach of vortices to riblets makes a significant contribution to surface stress of riblets.

Next, we investigate the relation between the riblet shape and the torque around the root of riblet, T^+. The superscript $()^+$ denotes the normalization with the frictional velocity and the kinematic viscosity. The correlation coefficients between T^+ and a streamwise variation of the relative spanwise displacement, h_z^+, and its streamwise derivative, dh_z^+/dx^+, are 0.16 and 0.88, respectively. This suggests that the riblet is subjected to the high surface stress where it deforms in a spanwise direction. Similarly, the correlation coefficients between T^+ and the height, h_y^+, and dh_y^+/dx^+ are respectively –0.57 and 0.57. Further study will reveal the statistical tendency of the torque and geometrical features of riblets with other shapes

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Flow field analysis around salt particle collection device of dry gauze method using porous media model

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Key Words: *Dry Gauze Method, Computational Fluid Dynamics, Porous Media Model*

Since airborne salt causes corrosion in steel materials, it must be evaluated for the management of steel structures. The dry gauze method, which uses a gauze embedded in a wooden frame, is often used to evaluate the amount of airborne salt. This method evaluates the amount of salt captured by the gauze while salty air passes through it. Although observation results using this method are abundant, the collection efficiency for salt particles has not been clarified owing to complex airflows around the device. Obata and Murakami [1] reported that the collection efficiency differed in each observation period and did not sufficiently explain the cause of this difference.

Therefore, to clarify the collection efficiency, the authors simulated the flow field around the device using computational fluid dynamics (CFD) with a large eddy simulation to estimate the collection efficiency with particle tracking. To represent a fine structure of the gauze fiber, a very fine computational grid is required, which is computationally expensive. Therefore, in this study, the gauze was modeled as a porous medium [2] to reduce computational costs. Wind tunnel tests were performed to obtain the pressure loss coefficients of the gauze, which are necessary for the porous media method.

In the research process, first, the flow field around the collection device was evaluated using visualization tests in a wind tunnel. Then, the flow field around the device was calculated using CFD and compared with the results of the flow visualization tests. The flow visualization tests showed that airflows were perpendicular to the gauze on the leeward side of the gauze, regardless of the wind direction. This is because the airflow is rectified when the airflow passes through the gauze with a small porosity. The flow fields around the device were reproduced well in all the wind directions investigated using the porous media model in this study, which considered the tangential resistance as well as the normal resistance of the gauze. This result suggests that the tangential resistance must be considered in the porous media model when the porosity of an object is small, even if the thickness is small. Then, particle tracking was performed to quantitatively evaluate the dependence of the collection efficiency on the wind speed and direction. The results indicated that the collection efficiency was affected by the complicated flow around the collection device.

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Flow Separation Control by Using Wave-like Body Force in Backward-facing Step Turbulent Flow

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Key Words: Backward-facing Step Flow, Reattachment Length, Traveling Wave Control, Body Force, Direct Numerical Simulation

Flow separation is a canonical phenomenon in fluid dynamics and fluid machinery. The phenomenon enhances heat transfer and fluid mixing while causing an increase in drag and noise pollution due to abrupt changes in pressure and flow rate. Therefore, controlling it is strongly required in engineering applications. In this study, we perform direct numerical simulations of backward-facing step turbulent flow with the traveling wave-like body force control. We chose the traveling wave to control the flow separation due to twofold reasons; Schäfer *et al.*[1] pointed out that the reattachment length is greatly oscillated by the separation bubble; Mamori *et al.*[2] reported that the traveling wave control enhances the mixing of the vortex. Therefore, we expected that the traveling wave enhances the separation bubble mixing and affects the reattachment length. Accordingly, the purpose of this study is to investigate the effect of control parameters on the reattachment length and to clarify the mechanism.

In the stationary wave (i.e., the wavespeed is zero), the separation bubbles became smaller and the reattachment length decreased as compared with those in the uncontrolled case. This was because the negative wall-normal velocity was induced by the body force in the downstream half of the step. Additionally, since the velocity fluctuation and the vorticity in the recirculation region decreased, the mixing of the separation bubble was suppressed. In the downstream traveling wave, the reattachment length decreased compared to that in the uncontrolled case and the stationary wave case. The velocity fluctuation and the vorticity in the recirculation region increased, which decreased the size of the separation bubble. Moreover, the separation bubble was oscillated and was released periodically. The phase analysis showed that this period was consistent with that of the traveling wave, which means that the traveling wave dominates the oscillation period of the separation bubble. The periodic component of the velocity showed that the traveling wave produced alternately slow and fast mainstream velocities on the step.

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Flow Structure Analysis Related to the Acoustic Wave Generation in Subsonic Free Jet Using Dynamic Mode Decomposition

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Key Words: *Aeroacoustics, Mode Decomposition, Flow Visualization*

In a subsonic free jet, a vortex sound is generated at the end of the potential core. However, the mechanism leading to the generation of vortex sound is still under discussion. A recent study proposed that pressure waves propagating upstream along the jet axis interact with Kelvin-Helmholtz (K-H) instability possibly forming a feedback loop that intensifies (Bogey, 2021) [1]. In this study, TlsDMD (Total least-square Dynamic Mode Decomposition) [2], a kind of Dynamic Mode Decomposition (DMD) [3], is applied to the time series of numerical results of an axisymmetric subsonic free jet [4], and a detailed analysis of this hypothesis is performed. In the study, the DMD mode at the K-H instability frequency, which is the dominant frequency peak near the nozzle exit, was extracted. From this result, we found that this DMD mode describes not only the K-H instability wave but also pressure waves propagating upstream along the center axis. Based on this result, we applied the Spatio-temporal Fourier analysis to detect the waves propagating upstream direction. As a result, we confirmed that they originate from the end of the potential core. In other words, there is a *feedback mechanism* at the frequency of the K-H instability. Then, our results support the presence of a feedback mechanism in a subsonic free jet. For the flow characteristics, there is a possibility that there exists an unstable global solution that takes the form of a feedback loop. This content is currently under investigation, and we believe that the mechanism can be elucidated by the time of the presentation.

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Interaction between Indoor and Outdoor Air Pollution in Natural Ventilating Building: Application to Sense-City urban area

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Key Words: *Air Quality, CFD, RANS, Sensitivity Analysis, Sense-City, Full Scale Experiment*

As majority of people spend 90% of their time in indoor environment, air quality has become an important scientific field in the last few decades. Indoor air quality is affected by many factors. One of the significant factors is outdoor air pollutions [1]. They enter the indoors through ventilation systems or natural ventilation and may stay indoors for a long time due to the airtightness of buildings. The present study especially focuses on nitrogen dioxide (NO2) concentration in a natural ventilating room that comes from outdoor pollutant source such as vehicle emissions.

In the present study, we have performed numerical simulations of a controlled environment in Sense-City urban area [2]. Sense-City is a unique full-scale equipment that can reproduce controlled conditions of temperature, humidity, airflow and pollution using an atypical climatic chamber. Reynolds Averaged Navier-Stokes (RANS) simulations have been carried out to calculate outdoor and indoor NO2 concentrations. RANS simulations are performed in two steps: district scale and building scale. Pressure values and pollutant concentrations are extracted from the district scale simulation and applied to the building scale simulation as boundary conditions. As expected, a sensitivity analysis study shows that the NO2 concentration in the building depends mainly on the pollutant concentration at the windows. Once opening windows, indoor pollutant concentration reached the almost same level of that of outdoor within a few minutes. Therefore, the interaction between outdoor and indoor air quality cannot be negligible for indoor air quality.

This study can be useful for engineers and for local authorities to understand the importance of considering the interaction of the indoors and outdoors, the potential and limitation of RANS simulation in a natural ventilating. Considering the limitation of the number of sensors for air pollution in real applications, CFD simulation is promising to obtain air pollutant distribution cartography. It can also be used as a decision-support tool for relevant urban planning such as the optimal placement of sensors and depolluting systems in urban areas.

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Investigation of Multi-phase-field Model without Lagrange Multiplier for Multiphase Flow Simulation

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Key Words: *Multiphase Flow, Multi-phase-field Model, Conserved Allen-Cahn Equation, Numerical Simulation*

Multiphase flow is a universally important phenomenon in science and engineering. Thus, there is a requirement to explore in detail the characteristics of multiphase flow. However, as the direct experimental observation of multiphase flow is difficult, numerical studies are indispensable to create a deeper understanding of multiphase flow.

The phase-field (PF) method is a powerful interface tracking model within the multiphase flow simulation, as it does not require explicit tracking of the interface position. The Cahn-Hilliard (CH) equation [1], which can conserve the liquid volume accurately, has been used extensively in the multiphase flow simulation. However, it requires small time increments as it reduces to the fourth order differential equation which is a significant drawback. To overcome this challenge, the conserved Allen-Cahn (CAC) equation [2] has been proposed, where a larger time increment can be utilized. Recently, the CAC model was applied by the authors to a multiphase flow with three or more phases by employing the multi-phase-field (MPF) method [3]. In the CAC-MPF model, the Lagrange multiplier method was introduced to model the interaction among the multiple PF variables. Although the CAC-MPF model successfully simulated the multiphase flow with an arbitrary number of phases, the degree of freedom in the selection of the Lagrange multiplier remains to be determined.

In this study, a new CAC-MPF model without the Lagrange multiplier was developed for multiphase flow problem. To this end, the MPF model developed by Steinbach [4] was modified, that is, the Lagrange multiplier was removed by introducing the concept of interface field. Further, the accuracy of the model was evaluated through numerical simulations.

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Investigation of Steam-Diluted Hydrogen/Oxygen Lifted Flame Formed with Cross Jets in a Multi-Cluster Burner

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Key Words: *Lifted Flame, Hydrogen Combustion, Steam dilution, Multi-Cluster Burner*

Hydrogen is expected as an alternative fuel due to its carbon free combustion features. The hydrogen combustion power plants which produce the stable output have an important role to realize hydrogen society. The thermal efficiency of a semi-closed gas turbine cycle designed for use in a cycle for hydrogen combustion power plants is expected to have higher than that of the combined cycle used in conventional thermal power plants [1]. A burner of the thermal cycle may burn pure hydrogen and oxygen diluted with steam. A diffusion flame configuration with multiple jets (referred to as a "multi-cluster burner") is considered to enhance mixing and avoid flame flashback since hydrogen combustion yields a high laminar burning speed. Also to further promote mixing, it is suggested that the jet ports are arranged in the combustor so that the jet flows impinge on each other.

DNS and experimental studies are investigated the combustion characteristics of a lifted flame formed in a multi-cluster burner, which consists of multiple jets where the fuel and oxidizer jet cores collide one another, which feed hydrogen and oxygen diluted with steam as fuel and oxidizer [2-5]. DNS study performed in the multi-cluster burner where two tilted oxidizer jets and one fuel jet are paired [2]. The present DNS study performed in the multi-cluster burner, which narrows the distance between the pairs and further enhances the interaction between them. The present study focuses on the investigation of the mixing and combustion characteristics of lifted flames formed cross jets in such a multi-cluster burner, and three-dimensional DNS of lifted flames formed in the multi-cluster burner has been performed and analyzed.

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Low-Dimensional Representation of Unsteady Flow based on CNN and LSTM

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Key Words: *Unsteady Flow, Machine Learning, CNN, LSTM, Low-Dimensional Representation*

Deep learning is expected to be one of powerful tools for understanding, predicting, and controlling nonlinear flow phenomena. For example, Guo et al. constructed an approximation model for real-time prediction of non-uniform steady laminar flow based on convolutional neural network (CNN) [1]. Hasegawa *et al.* proposed a method to construct a machine-learned reduced order model for unsteady flows by combining a CNN autoencoder and a long short-term memory (LSTM) [2].

In this study, we build deep learning models with CNN and LSTM architectures to develop low-dimensional models to represent unsteady flows. As an example of unsteady flows, direct numerical simulation of a flow around a cylinder at Reynolds number $Re_D = U_\infty D/\nu$=100 is carried out to obtain a time-series data of the flow field for training and validation. Three types of the models have been constructed: Conv3D Model, Conv2D+LSTM Model and CNN Autoencoder (AE) Model. For Conv3D Model and Conv2D+LSTM Model, previous time series data of the flow field are given as input, and the flow field at the next time step are predicted as output. Conv2D+LSTM Model apply Convolutional 2D Layer for spatial dimensional reduction and LSTM Layer for time advancement in a sequential manner. Conv3D Model utilizes Convolutional 3D Layer to perform dimensional reduction in both space and time and output the flow field at the next time step in a batch processing. To obtain a time series of the flow field, time advancement is achieved sequentially in both Conv3D Model and Conv2D+LSTM Model. For CNN AE Model, a time series of the flow field for almost one cycle of the vortex shedding are given as input. The model applies Convolutional 3D Layer for dimensional reduction and extension in both space and time. The model then reconstructs the input as output approximately. CNN AE Model output a time series of the flow field in a batch process.

The flow fields predicted by all three models agree qualitatively and quantitatively with the ground truth obtained by numerical simulation of the flow (CFD), in terms of instantaneous distribution of the flow field, correlation coefficients and mean square of error between the prediction and the ground truth, and power spectrum of velocity. Compared with Conv3D Model and Conv2D+LSTM Model, CNN AE Model with only 1 mode, 2 or 3 modes in the latent space gives better agreements with the ground truth. Conv2D+LSTM Model showed the largest errors due to a phase shift. These differences of the model prediction can be explained by characteristics of the model architectures. The sequential processes for time advancement tend to accumulate larger phase shift errors, compared with batch processes with convolution operations. It is indicated that a reduced order model with only a batch process by the convolution operation could provide robustness against errors due to a phase shift. CNN AE Model with 2 modes in the latent space predicts the flow field better than the model with 1 mode or 3 modes. The two-dimensional unsteady flow around a cylinder can be represented with high accuracy by only 2 modes in the latent space.

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Microfluidic Multiphase Flow Simulation Using an Advanced Diffuse-interface Model-based Method

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Key Words: *Computational Fluid Dynamics, Multiphase Flow, Phase-field Method, Diffuse-interface Model, Conservative Level-set Equation, Lattice Boltzmann Method.*

For developing and evaluating microfluidic devices in various fields of science and engineering, we construct computational fluid dynamics (CFD) methods based on a phase-field model [1] and its extended version of a multi-phase-field model [2] to simulations of incompressible multiphase flows. For calculations of diffuse-interface advection and autonomous formation in the flow, both the CFD methods adopt a conservative Allen-Cahn (CAC) [3] equation instead of Cahn-Hilliard (CH) equation [4]. The AC form is advantageous over the CH form in terms of computational efficiency, interfacial tension effect and volume conservation because the former is free from curvature-induced diffuse-interface drift motion and it has a second-order differential diffusion term instead of the fourth-order term in the latter. A semi-Lagrangian formed lattice Boltzmann method (LBM) [1,5] is employed as a 2^{nd}-order numerical scheme for solving the Navier-Stokes equations with the AC equations. The LBM is useful for high-performance computing because of simple and conservative pseudo-particle kinematic operations on an isotropic spatial grid [5]. From numerical results of droplet motions it is confirmed that the methods would be applicable to complex multiphase systems with partially wetted and 3D micro/nano structured surfaces [6,7].

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Modeling of PM2.5 Deposition Behavior on the Wall Surface

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Key Words: PM2.5, Deposition behavior, Image force, Lagrangian particle tracking

In order to reduce various health risks due to aerosol particles, it is of great importance to analyze the behavior of aerosol particles. Especially, the health risk of PM2.5 are greater than those of larger particles sizes[1, 2]. Therefore, in the present study, we investigate the deposition behavior of PM2.5 by means of a direct numerical simulation. In the present simulation, we consider two different flow: a turbulent channel flow and a square duct flow. In turbulent channel flow, the amplitude of the applied voltage for particles deposition increases as the particles sizes increases. On the other hand, influence of the mirror image force is so small. In a square duct flow, which is similar flow geometry in the experimental study[3], we investigate the influence of the inlet flow and the particle size for the particle deposition. Similar to their experiments, the amount of the particle deposition increases as the particle size decreases and the inlet flow decreases. In the cases of smaller particle sizes, particles cannot follow the flow due to the Brownian motion. In the case of large inlet flow rate, the inlet flow make the particles separated from the flow, and they collide with the wall surfaces in the outlet plane. Therefore, many particles are deposited on the wall in the outlet plane. In the final presentation, we will show the results by the further investigation, i.e., the deposition behavior in junction flows.

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Neural-network-based estimator for turbulent flows from limited heat information

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Key Words: Neural Networks, State estimation, Turbulent flow

Understanding of internal combustion phenomena is important for achieving high-efficiency engines; however, it is difficult to measure the detailed thermo-fluid phenomena directly. To tackle this issue, we aim to estimate physical quantities in internal combustion engines from wall sensor measurements. We here utilize neural networks for the estimation. Neural networks have become an indispensable tool and covered a wide range of fluid problems, such as flow control and enhancing simulation [1]. State estimation is not an exception. Many researchers have estimated the flow field from limited sensors with neural networks. In many of the previous attempts, the wall shear stress and the pressure are commonly used for the input attribute of neural networks [2, 3]. However, considering the practical measurement for engine combustion, it is favorable to use the wall heat flux for the input. Hence, we here estimate near-wall physical quantities from the wall heat flux using a convolutional neural network (CNN). As an example, we consider a turbulent channel flow at the friction Reynolds number $\mathrm{Re}_\tau = 180$ and the Prandtl number $\mathrm{Pr} = 0.71$. The CNN estimates three-dimensional velocity and temperature fields from sensors on the entire wall. In the region near the wall, the estimated streamwise velocity and temperature are in reasonable agreement with the reference direct numerical simulation data. Furthermore, towards the practical application, we aim to estimate from a smaller number of sensors. We investigate the dependence on the streamwise and spanwise spacings of sparse sensors on the wall. At last, we consider the utilization of time-series wall measurements as input data to improve the estimation accuracy. In the talk, we will show the statistical assessments on these estimation attempts.

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Numerical Investigation of Solidification Process of Impinging Supercooled Water Droplet using Explicit Moving Particle Simulation

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Key Words: *Solidification, Droplet Impingement, Supercooled Water Droplet, Aircraft Icing*

Icing on an aircraft degrades flight safety; it is important to develop the prediction method of the icing. Although many icing simulation methods have been proposed [1-3], it has still been difficult to predict the supercooled large droplet (SLD) icing because the SLD icing involves complex phenomena composing of splash and bounce of the droplet and runback of the water film. We proposed a coupling method [4] of a grid-based method for airflow and a particle-based method for droplet behavior to predict the SLD icing. However, it is still difficult to apply the SLD icing because the freezing process of the supercooled water droplet is complicated due to the nucleation of the ice. This study performs the numerical simulation of SLD impinging and solidifying on the cold substrate and compares the solidification model of the release of supercooling to apply the coupling method.

The numerical simulation of SLD icing is performed by explicit moving particle simulation (E-MPS) [4,5]. The governing equations are composed of incompressible continuity, Navier-Stokes and energy equations. These equations are discretized by using the weight function, and the pressure is estimated explicitly. The substrate temperature is set as a constant temperature which is the same as the temperature of initial supercooled droplet.

For the impinging droplet icing, we compare two cases. One is the model that the solidification occurs at the surface of the wall, then the mixture (mixed-phase between water and ice) appears within a certain thickness. The other model is that all particles composed of the droplet change into the mixture phase just after the impingement, i.e., the release of supercooling for all components inside the droplet instantly occurs after the impingement. For both cases, the substrate temperature is assumed to be constant, and we neglect the heat transfer from the droplet to the surrounding air. As a result, we confirmed that the solidification occurs from the near wall to the location apart from the wall for both cases. Then, the total solidification times are comparable for both cases, indicating the availability of the model. At the conference, we will show the results of aircraft SLD icing using these models.

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Numerical Simulation of Droplet Impingement on Wall with Thin Liquid Film by E-MPS Method

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Key Words: *Droplet impingement, Moving Particle Simulation, Liquid film*

Ice accretion is a phenomenon in which supercooled droplets or ice particles in the atmosphere impinge on a solid surface, and an ice layer is formed there. The ice accretion on an aircraft threatens the navigation safety because it causes deformation of the wing shapes and reduces aerodynamics performance. Hence, it is very important to predict icing at the design phase of an aircraft. In the glaze ice conditions, where the temperature is relatively high, impinged droplets do not freeze instantly and they runback along the airfoil as a liquid film. As a result, they form characteristic icing shapes, such as a horn. In addition, when supercooled large droplets (SLD), which has more than 40 μm diameter, impinge on an aircraft and they acconpanied by splash and rebound. Therefore, the physics is so complex and the prediction is very difficult. The purpose of this study is modeling the droplet impact behaviour on a thin liquid film in terms of SLD icing by using the three-dimensional E-MPS method.

Moving Particle Semi-implicit (MPS) method[1] is a Lagrangian approach based on the governing equations at the motion of each particle. It is a meshless method and suitable for analyzing phenomena with large deformations of interface between multi-phase fluids. In addition, MPS method strictly satisfies the conservation of mass. Furthermore, explicit moving particle simulation (E-MPS) method[2] is faster than ordinally MPS method because of the explicit pressure solver. In this study, we used E-MPS method with the incompressible Navier-Stokes equations and the mass conservation equation (i.e. continuity equation) as the governing equations.

In the present study, a water droplet of 1.95 mm diameter impinges on a wall at velocity magnitude of 3.75 m/s. On the wall a water film with 0.434 mm thickness exists. As the impact angle was changed is changed from 90 to 15 degrees. When the droplet impinge vertically, the crown is formed by the impingement, and no secondary droplet is generated by the finger jets. As the impact angle reduces, the crown width in the direction of droplet movement increases significantly, and secondary droplets from the finger jets are generated. However, the crown width perpendicular to the direction of droplet movement and the crown height slightly change. When the impact angle reduces more, the crown height decreases and finally the crown cannot form and the droplet coalesces into the water film.

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Numerical simulation of interaction between two Savonius turbines aimed at practical application of ocean current power generation

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Key Words: *Savonius type turbine, numerical simulation, rotating object, domain decomposition, incompressible flow, ocean current power generation*

Renewable energy is important as a way to solve global warming and energy problems. In this study, we investigate the flows around two Savonius turbines that rotate independently by numerical simulation considering the application of ocean current power generation since the stability of the entire device can be improved by rotating two devices side by side in the opposite direction. This drag type device is chosen considering that the speed of the ocean current is small.

In general, when analysing the flow around a rotating object, a rotational coordinate system is often used. However, it is difficult to calculate with such coordinate system when two objects rotate in the reverse direction independently.

Therefore, in this study, the entire area was divided into a plurality of rectangular areas including one rotating device. At this time, data is exchanged between each area through the sides of each rectangle. One rectangle is divided into an inner circular area and an outer circular hollowed out rectangular area. In the circular area, the rotating coordinates matched to the rotation of the rotating device were used, and in the external area, the stationary coordinate system was used. Since the data in the two areas are passed on the circumference, not only the calculation time required for interpolation is significantly shortened, but also the accuracy of interpolation is improved. The internal region is further divided into several regions in order to generate a grid along the blade of the Savonius type rotating device.

In this method, since an independent rotating coordinate system is used in each region, the rotation speed of the rotating device can be freely changed for each rotating device. Further, this method can be applied regardless of the number of rotating devices. This time, using this method, the flow was calculated for the case where two rotating devices rotate in opposite directions and in the same direction.

The basic equations are the incompressible Navier-Stokes equations expressed by the both rotational and stational coordinate systems. The nonlinear terms of the basic equations are approximated by the third order upwind difference in order to perform stable calculations even at high Reynolds number. The fractional step method is employed to solve the basic equations.

The calculation was performed by changing the angle of attack, the rotation speed of the rotating device, the distance between the devices, etc., and the influence on the torque and power was investigated together with the analysis of the flow field.

It was found that the total value of the torques of the two units may be maximized when the flow hits the line connecting the center of the rotating devices at an angle of 45 degrees. The calculations were performed not only by fixing the rotation speed of the rotating device, but also by changing the rotation speed according to the torque acting on the rotating device where the Newton's equation of motion for the device was solved.

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Validation of a New 2-scalar Flamelet Approach of LES for Turbulent Combustion

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Key Words: *Turbulent Combustion, Large Eddy Simulation, Flamelet Approach*

Large Eddy Simulation (LES) is a promising tool for predicting the combustion field when fluid dynamics and flame instability are encountered. Among the turbulent combustion models for LES, Kim[1] has proposed a new 2-scalar flamelet approach. It is based on a generalized theory of fluid interface which combines a conservation law of thermodynamics and the solution of a viscid level-set equation. To deal with the combustion problem, a conservation scalar, mixture fraction, is used to represent the global outer flame condition by referring to a distinct 0-dimensional detailed chemical reaction solution based flamelet database in which the equilibrium state characterizes the corresponding mixture composition, and a level-set of non-dimensional sensible enthalpies as a chemical progress indicator determines the inner flame structure by evaluating the conventional level-set variable G with a local burning velocity model[2] which explicit the diffusion term in a finite flame thickness. This study extended Kim's approach to the turbulent LES. Due to the non-empirical flamelet database, one just needs to alter the laminar burning velocity used in the burning velocity model to a turbulent one which is calculated by an experimental correlation[3]. To quantitively evaluate this new approach's prediction accuracy, a typical turbulent partially premixed combustion field, Sandia Flame D, is chosen as the validation target. This simulation is performed by the FrontFlow/red, and the computational grid comprises 21,388,608 hexahedral unstructured elements which are parallelly processed by 288 cores. The annular pilot jet inlets are constructed by simplified geometries. By furtherly introducing a premixed flame after these inlets, an experimental turbulent intensity at the burner exit is generated. Different from other simulations using this fluctuation as the inlet velocity condition, these robust turbulence motions improved the prediction accuracy of the velocity field at the regions after the burner exit. At all measuring sections of the combustion field, Kim's approach indicates good agreement with the experiment. At the fuel-lean and rich regions where the burning velocity is low, an extra diffusion term of the level-set equation uniforms the distribution of sensible energy, which led to an experimental tendency at those two regions. However, at the stoichiometric region, the simulation results overestimate the experiment slightly. The reason is that the flamelet database for LES requires an accurate turbulence diffusion resolved by grid scales at the inner flame region though it has already included a sub-grid scales diffusion model. Nevertheless, by comparing with the results of a recently released paper [4] in which the gird resolution is 15 times this one, the results of this study have a considerable degree of accuracy.

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A Thermodynamically Consistent Constitutive Model Coupling Diffusion, Reaction and Deformation for Biodegradable Polymers

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Key Words: Chemo-mechanics, Multiphysics Couplings, Large deformations, Finite elements

Biodegradable polymers are a class of polymers that break down after fulfilling their intended function. This unique property makes them very promising in healthcare applications such as sutures, stents, and scaffolds, as the need for retrieval surgery is completely eliminated. In this context, modelling of hydrolysis degradation in polymers is critically needed in view of accelerating device development. However, understanding the factors that affect the device performance and service life under complex environment remains limited. Great challenges remain in modelling the response of these materials due to the presence of highly coupled phenomena [1]. Early models either mainly focused solely on developing kinetics of hydrolytic degradation or examining the degradation of mechanical parameters using semi-empirical approaches and experimental tests. Only few very recent studies modelled the mechanical behaviours. However, these studies are incomplete in considering the diffusion of water or reaction products.

This study try to fill this gap by developing a general thermodynamically consistent constitutive framework for degraded polymers that couples water and short soluble chains diffusion, hydrolysis reaction, and large deformation. In the constitutive framework, the state-of-the-art kinetics of the hydrolysis reaction considering the effects of auto-catalysis and stress-enhanced reactivity have been incorporated in the continuum model in a consistent manner [1]. The constitutive equations for the stress, chemical potential, and dissipative driving force are derived by means of the reduced entropy inequality [2, 3]. The model is implemented in the finite element framework for solving representative problems with simple geometries. A general implementation is also proposed through an ABAQUS user-defined subroutine. The numerical results suggest that the developed model can predict the coupled phenomena and reveal the effects of design factors on the degradation process. We hope our constitutive framework and presented results would enable the rational design of biodegradable polymer materials and devices under possible service environments.

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Crease Nucleation and Propagation from a V-shaped Notch in an Elastomer

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Key Words: *Surface Instability, Creasing, Wrinkling, Nucleation, Propagation, Elastomers*

We investigate crease nucleation and propagation from a V-shaped notch in an elastomer. Plane strain finite element analysis is performed considering the isotropic thermal expansion of an incompressible neo-Hookean solid (e.g., swelling can be mimicked by thermal expansion). The nucleation of the first crease occurs at a global compressive strain ε_{G1}, which decreases from $\varepsilon_{wrinkle}$ to zero as the notch depth increases (i.e., ε_{G1} causes mesh dependence). Here, $\varepsilon_{wrinkle}$ is the critical compressive strain for wrinkling while ε_{crease} is defined as the critical compressive strain for creasing [1–3]. The propagation mechanisms of sequential creases are analysed by self-organization and nonlinear perturbation approaches, leading to finding a threshold compressive strain $\varepsilon_{threshold}$. These three critical compressive strains are in the relation of $\varepsilon_{crease}<\varepsilon_{threshold}<\varepsilon_{wrinkle}$. The case of $\varepsilon_{G1}<\varepsilon_{threshold}$ predicts the crease propagation regularized at $\varepsilon_{threshold}$ whereas the case of $\varepsilon_{G1}>\varepsilon_{threshold}$ is supercritical. The former case (i.e., $\varepsilon_{G1}<\varepsilon_{threshold}$) allows a nonlinear perturbation to nucleate a sequential crease at an arbitrary place by overcoming an energy barrier [4]. The self-organization approach predicts narrow crease distances, which are different with the crease distance that minimizes the elastic energy. The critical crease distance is broader and increases sensitively approaching to $\varepsilon_{threshold}$ but the energy difference is slight.

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Investigation of the Linear Viscoelastic Property for Polyacrylamide Hydrogels during Transient Equilibrium Swelling

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Key Words: *Polyacrylamide hydrogels, Transient equilibrium swelling, Viscoelasticity*

The present study experimentally examines the linear viscoelastic property of polyacrylamide (PAAm) hydrogels during transient equilibrium swelling. To this end, we conduct dynamic mechanical analysis on various specimens with different monomer and cross-linker concentrations. The transient equilibrium swelling is replicated using specimens with different water contents at the equilibrium state. The swelling-dependent linear viscoelasticity based on the scaling theory[1] is originally formulated to support the theoretical discussion of measured results.

The elastic moduli of PAAm hydrogels follow the scaling theory during the swelling from the as-prepared state, yet they change more complex during the de-swelling process. To be more specific, although the elastic moduli of PAAm hydrogels with a high monomer concentration also follow the scaling theory[2], those with a low monomer concentration irregularly change for the volume swelling ratio. Further, they eventually converge to a characteristic value independent of the monomer and cross-linker concentrations at the sufficiently de-swelling state named the extreme state.

The relaxation times of PAAm hydrogels at the extreme state have a characteristic value, and thus their viscoelastic property is uniquely determined regardless of their constituents. The viscosity during transient equilibrium swelling does not follow Newton's law of viscosity; in particular, by the swelling, a PAAm hydrogel with a high cross-linker concentration behaves more elastically, yet the viscosity increases.

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Modelling liquid penetration and hygro-expansion in paper

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Key Words: *porous-fibrous material, multiscale modelling, out-of-plane bending, curl*

Paper, a hydrophilic material, is susceptible to deformations due to variations in moisture content which develop over time [1]. Understanding the moisture transport through the thickness of a paper sheet and the resulting time-dependent mechanical response allows us to predict the curling behaviour of paper [2,3].

In this work, the time-dependent factors involved in the deformation of a paper strip that is fully or partially wetted from one side and subjected to different boundary conditions is studied with a one-dimensional numerical model. The different time scales involved, in the process of imbibition in the inter-fibre pores and absorption (or water uptake) by the fibres, are analysed. The resulting hygro-expansion due to swelling of the wet fibres is then solved to predict the bending response of the paper strip due to the non-homogeneous through-thickness moisture distribution. We provide a phenomenological model here to describe the dynamic water flow through the thickness of the paper strip, via the pores, using the unsaturated flow theory. The pore-fibre water exchange is modelled as a diffusion process dependent on the wetted pore surface area. The resulting moisture-induced displacements are characterised through a hygro-elastic material model.

The numerical analysis shows a fair agreement with experimental observations. An independent immersion test provides us with an estimate of the time scales involved in the liquid transport, which is then used to characterise the curling response of the paper strip.

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Modelling of Bicontinuous Metal-Polymer Composite Actuators

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Key Words: *Composite Actuators, Electroactive Polymer, Chemo-electro-mechanical Coupling, Transport Modelling*

Electroactive polymers are well known for their large strain response under electrical stimulus, which can be utilized for actuation applications. However, for extensive mechanical use in electro-mechanical systems, they lack the necessary strength and stiffness. It has been proposed to utilize metal reinforcements to increase this stiffness, while ideally maintaining large actuation strains.

Here, we consider an interpenetrating metal-polymer composite actuator consisting of a ionically activated polymer and a nanoporous metal skeleton. The nanoporous metal exhibits a unique bicontinuous microstructure [4] that facilitates mechanical support as well as almost unhindered ion flow in the solvent-saturated polymer phase. The composite shows increased actuation strains while still retaining the metal's superior mechanical properties [2].

In order to exploit the full potential of these nanocomposite actuators, a detailed understanding of the underlying structure-property relationships and means to predict the actuator's response are necessary. Using continuum mechanical modelling and finite element simulations, the mechanical properties of this nanocomposite as well as it's functional behaviour are investigated [1,3,5]. It can be shown that by modification of the nanocomposite's structure, transport paths, mechanical properties and reaction times can be altered significantly, thus, providing the means to tailor the actuator behaviour to different applications.

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Morphological Evolution of Surface Patterns in Hydrogel Bilayers

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Key Words: *Surface Instability, Wrinkles, Hydrogels, Swelling, Polyacrylamide*

We study the morphological evolution of surface patterns in polyacrylamide (PAAm) hydrogel bilayers comprising a thin stiff film on a thick soft substrate. A pre-gel solution of acrylamide in water is poured onto the hydrogel substrate and left in air for a prescribed period of time to allow the solution to become a hydrogel film bonded to the substrate. During the gelation process, hexagonally packed dimples form on the surface, which then evolve into randomly oriented wrinkles. We presume that the mechanism of the formation and evolution of the patterns is twofold. First, the film constrained by the substrate swells owing to uptake of water molecules from both the substrate and an uncured liquid layer present on the top surface in contact with air, thereby experiencing an in-plane equi-biaxial compressive stress. Once the stress exceeds a critical value, the surface instability occurs, resulting in the formation of hexagonal dimples. Second, as the swelling proceeds, the magnitude of applied stress in relation to the critical stress, or overstress, in the film increases, causing the dimples to transition into wrinkles [1]. We find that the wavelength decreases during the pattern evolution and remains nearly constant once the wrinkles form. Furthermore, the wrinkle wavelength can be controlled in the millimeter-scale range by adjusting the film thickness. The formation and evolution of the patterns described above are due to coupling between solvent transport and deformations. Our findings offer a route to fabricating large-scale wrinkles in PAAm hydrogels.

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A Gaussian process based Bayesian optimization calibration approach and its application in terradynamics

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Key Words: Gaussian process, Bayesian optimization, Terradynamics, Smoothed particle hydrodynamics, Semi-empirical soil contact model

We seek to accelerate terradynamics simulations with interaction to solid bodies by using an semi-empirical soil contact model (SCM) [1] with a few simulation parameters that can be calibrated from experiment data or high-fidelity simulation data. To this end, the Gaussian process (GP) based Bayesian optimization (BO) approach [2] is employed in this work. First of all, to get the high-fidelity simulation data as the "ground truth" in the calibration step, a more accurate continuum model based on the Smoothed Particle Hydrodynamics (SPH) method is employed [3]. The deformable terrain is modeled as an elasto-plastic continuum and discretized with SPH particles that dynamically interacts with the solid bodies in a co-simulation setup. The interaction between the solid body and the deformable terrain is handled through so-called boundary conditions enforcing particles. Several simulations are performed using the SPH model to obtain the "ground truth" data. Second, an initial guess of the SCM parameters (7 parameters in this work) is chosen according to experience, and used to run the SCM simulation. The SCM simulation result is then compared with the "ground truth" and use the GP-based BO approach to find the distribution of the next possible set of parameters that can be used to run the following SCM simulation. Finally, the above operation steps will iterate for several times until a set of SCM parameters is found, with which we can get a simulation result that matches the "ground truth" best. Both the SCM and SPH simulations will be performed in an open-source software called Chrono. The GP-based BO will be performed in an separate package by using Python scripts to interactively communicate with the developed terradynamics solver.

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Continuum simulation for granular silo discharge flow using a regularized non-local $\mu(I)$ model

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Key Words: *Dense Granular Flows, Silo Discharge, Non-local Effect, $\mu(I)$ Rheology*

In this work, we implement the non-local rheology [Bouzid *et al.*, Phys. Rev. Lett. **111**, 238301 (2013)] into a well-developed continuum flow solver [Lin and Yang, J. Comput. Phys. **420**, 109708 (2020)] to simulate the two-dimensional granular silo discharge flow. The discharge dynamics of non-local simulation show qualitative agreement with the particle-based simulation data and the continuum simulation using local $\mu(I)$ rheology [Staron *et al.*, Eur. Phys. J. E **37**, 5 (2014)], while the non-local effect enhances the volume discharge rate compared to the local model prediction when the silo orifice is narrower. Thus, we examine the difference between the local and non-local flow rate versus the silo orifice size, a monotonically growth of flow rate difference with decreasing orifice size is revealed, independent of silo aspect ratio and model parameters. Finally, we evaluate the time evolution of high-shear zone during discharge process and find the non-local momentum transport facilitating the flow over a wider domain to increase the flow rate for the narrower orifice.

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DEM Simulation of Particle Mixing in Horizontal Stirred Bed Reactors

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Key Words: *Horizontal Stirred Bed Reactors (HSBRs), Mixing, Discrete particle model*

Horizontal stirred bed reactor (HSBR) is a type of reactor for axial powder mixing whose use in gas-phase polymerization of, e.g., polypropylene, has grown significantly in recent years [1]. The reactor usually has a bed of particles that is gently agitated by a series of paddles that are connected to a central shaft of the reactor.

In this work, we simulated the mixing of particles in an existing model of industrial HSBR based on a discrete particle model using the open-source software MercuryDPM [2]. The goal was to analyze the mixing process in terms of axial dispersion and mixing quality and determine the number of rotations required for efficient mixing. This process was analyzed by investigating different properties, including cycle time, Lacey index, and axial dispersion coefficient. First, the cycle time distribution was obtained by tracking the particles, and the result was validated using coarse-graining [3]. We obtained the Lacey mixing index using particle tracking and found the minimum number of rotations needed for efficient mixing. Finally, we measured axial dispersion, where we observed sub-diffusive behavior in the mixing process.

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Lethe: Open-source high-order unresolved and resolved CFD-DEM based on the deal.II library

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Key Words: *Discrete Element Method, Unresolved CFD-DEM, Resolved CFD-DEM, Multiphase Flow, Finite Element Method, High-Order Methods.*

Resolved and unresolved CFD-DEM couple CFD for the fluid phase with the Discrete Element Method (DEM) for the solids. Unresolved CFD-DEM solves the volume-averaged Navier-Stokes equations for the fluid at a scaler greater than the particle dimension and uses DEM to simulate the solid phase. Several particles occupy the same mesh cell. The two phases are coupled using expressions for the hydrodynamics forces (e.g., drag). Resolved CFD-DEM is more accurate than unresolved CFD-DEM because it fully accounts for the flow around each particle without additional models to couple the particle and fluid phases. Both approaches are complementary. Resolved CFD-DEM enables a deeper understanding of particle-fluid interaction whereas unresolved CFD-DEM can be used to accurately simulate processes at the pilot scale.

In this work, we introduce Lethe [1], a monolithic, open-source high-order unresolved and resolved CFD-DEM solver. Lethe solves the incompressible Navier-Stokes and volume-averaged Navier-Stokes equations by applying a stabilized continuous Galerkin Finite Element discretisation. It is built upon the well-established deal.II library. Through its deal.II heritage, Lethe is able to handle large meshes (>1B cells), supports dynamic mesh adaptation and is based on a solid C++ architecture. Lethe possess a full DEM module[3], which, coupled with it's CFD capabilities, enable the simulation of solid-fluid flows using both resolved and unresolved CFD-DEM strategies.

First, we present the implicit CFD solver of Lethe. We discuss how the solver is extended to resolved CFD-DEM using a high-order implicit sharp-edge immersed boundary approach. We demonstrate the accuracy of the solver using the method of manufactured solutions and demonstrate its capabilities by simulating the dynamic of sedimentation spheres. We present the unresolved CFD-DEM capabilities of Lethe. We present our implementation of a stabilized high-order formulation for the VANS equation. Using the flows in liquid and gas fluidized beds, we validate the capabilities of Lethe to predict complex solid-fluid flow dynamics under a wide range of regime. This presentation aims at giving an overview of our efforts to produce a state of the art, fully open-source high-order CFD-DEM code which will enable the simulation of complex solid-fluid both at the particle scale and at the process scale.

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MercuryDPM: Fast, flexible, particle simulations

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Key Words: *Granular materials, DEM, DPM, MercuryDPM, Open-source*

We introduce the open-source package MercuryDPM, a code for discrete particle simulations, that we are developing. It simulates the motion of particles, by applying forces and torques that stem either from external body forces, (e.g. gravity, magnetic fields, etc...) or from particle interaction laws. For granular particles, these are typically contact forces (elastic, plastic, viscous, frictional).

MercuryDPM is an object-oriented C++ algorithm with an easy-to-use user interface and a flexible core, allowing developers to quickly add new features. It is parallelised using both MPI and OpenMP and released open-source under the BSD 3-clause licence. Its developers' community has developed many features, including moving (wearable) curved walls (polygons, cone sections, helices, screw threads, level-sets, nurbs, triangulated, etc); state-of-the-art granular contact models (wet, charged, sintered, melting, cohesive, etc); specialised classes for common geometries (inclined planes/chutes, hoppers, etc); non-spherical particles (multisphere, superquadric, bonded particles, deformable clusters); general interfaces (particles/walls/boundaries can all be changed with the same set of commands); liquid droplet/spray models; STL readers for industrial geometries; restarting; visualisation (xBalls and Paraview); a large self-test suite; extensive Doxygen documentation; and numerous tutorials and demos.

For efficiency, it uses an advanced contact detection method, the hierarchical grid. This algorithm has a lower complexity than the traditional linked list algorithm for polydispersed flows, which allows large simulations with wide size distributions.

It also contains a coarse-graining tool: MercuryCG, which is both integrated and usable as a stand-alone tool. Coarse-graining is a novel way to extract continuum fields from discrete particle systems. It ensures by definition that the resulting continuum fields conserve mass, momentum and energy, a crucial requirement for accurate coupling with continuum models. The approach is flexible and the latest version can be applied to both bulk and mixtures; boundaries and interfaces; time-dependent, steady and static situations; and, even experimental data. It is available in MercuryDPM either as a post-processing tool, or it can be run in real-time, e.g. to define pressure-controlled walls.

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Multiscale modelling of granular materials – Calibration of discrete particle models

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Granular materials are the most common type of raw material in industry, after water. A multitude of industries, such as mining, agriculture, food, pharma, manufacturing and construction, depend on processes involving granular materials. They are also common in many natural phenomena, from dune formation, soil erosion and water management to natural hazards, such as avalanches or volcanic deposition.

To develop trustworthy models for granular materials, one has to understand their behaviour on multiple scales: On the micro-scale, one has to understand the properties of single particles (their size, shape, density) and the contact behaviour of particle pairs (interparticle friction, cohesion, and elasto-plasticity). These properties in turn influence the granular behaviour on the macro-scale.

We have developed a multiscale model for granular materials, combining the Discrete Particle Model (DPM, aka DEM) with an application-specific continuum model (CM). Starting from simplified particle and contact models, DPM captures the collective behaviour of a granular material by simulating the movement of the individual grains. Bulk properties are then extracted from the DPM simulations and coupled to the continuum model.

To calibrate a DPM model, developers often use analytic relations between the micro- and macro-parameters that are either phenomenological or derived from contact mechanics. Alternatively, they use numerical studies, where hundreds of simulations are run for different parameters to develop a mapping between the micro and macro parameters. However, both approaches are not feasible for complex industrial materials, where wide particle size distributions, agglomeration, inclusion of liquids, sintering, drying, and other phenomena require complicated contact models with many micro-parameters.

To deal with these issues, we have developed an automated calibration technique: First, we measure the basic material parameters (e.g., particle size distribution, material density) and apply them directly to the discrete particle simulation. Next, we select standard bulk experiments (heap test, rotating drum, ring shear cell) appropriate for the process we want to model. We simulate the same processes in MercuryDPM [1] and measure the response of the simulated material. Then we apply a numerical optimisation algorithm to find the micro-scale parameters for which the response of the experiments and simulations match. This optimization is done using a probabilistic optimization technique as implemented in the open-source code GrainLearning [2].

We have preliminary data suggesting that this technique and methodology works, in fact it has already been used in several projects, yielding good results. The technique can find local optima in only two to three iterations, even for complex contact models with many microscopic parameters. We present several case studies, discuss the strengths and weaknesses of the technique, when and why it fails and when it does succeed.

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NextGen Chrono::GPU: An Open-Source Multi-GPU DEM Simulator with Complex Geometry Support

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Key Words: DEM, GPU, Complex Geometry, Open-source, Chrono

In this contribution we report the numerical features and development status of our open-source multi-GPU Discrete Element Method (DEM) simulation package, the next-generation upgrade of the existing simulator Chrono::GPU [1]. This package provides complex grain geometry support through clumped spheres. While the largest DEM simulation to date ran on **tens of thousands** CPUs with two billion particles, our simulator scales to hundreds of millions particles on **two** GPUs. To achieve this high efficiency without compromising the paramount accuracy requirement that defines challenging simulations, we employ the following salient numerical techniques:

- Using compressed integer-based data structures and just-in-time compiling to reduce memory footprint;
- Leveraging CUB (an efficient CUDA utility package) functions;
- De-coupling kinematic (such as contact detection) and dynamics computations (such as computing contact forces and numerical integrations) to split the workload onto multiple GPUs.

This package provides APIs to interface the multi-physics simulation engine Chrono [2], allowing co-simulations with complex mechanical systems, such as rovers operating on granular terrains.

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A mesh-insensitive finite volume solver: from compressible to incompressible flows

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Key Words: *Finite volumes, Flow Problems, CFD, Incompressible Limit*

Finite volume (FV) methods are ubiquitous in CFD simulations of industrial problems because of their robustness and efficient implementations. A drawback of existing cell-centered (CCFV) and vertex-centered (VCFV) strategies is their need for high-quality meshes, whose generation is extremely expensive in terms of man-hours of specialized technicians. Indeed, the accuracy of both CCFV and VCFV is compromised in the presence of distorted and stretched cells [1]. On the contrary, the face-centered (FCFV) rationale proposed in [2-6] provides a framework less sensitive to mesh quality, preserving the accuracy of the approximation even in the presence of complex unstructured meshes with highly distorted and highly stretched cells. The FCFV method defines unknowns at the face barycenter and uses hybridization to eliminate the degrees of freedom inside each cell. In addition, Riemann solvers are defined implicitly within the expressions of the numerical fluxes [6]. The resulting methodology provides first-order accurate approximations of the viscous stress tensor and of the heat flux, without the need of any gradient reconstruction procedure. In addition, FCFV is capable of constructing non-oscillatory approximations of sharp discontinuities, without resorting to shock capturing or limiting techniques. For flows at low Mach number, the method is robust and is capable of computing accurate solutions in the incompressible limit, without the need of introducing specific pressure correction strategies. Moreover, this strategy has been tested for a large variety of elements including prims and pyramids. Note that hexahedra with non-planar faces, where standard FV require a special treatment, can also be used. Numerical simulations of 2D and 3D benchmarks of external flows will be presented to validate the methodology in different flow regimes, encompassing compressible and incompressible flows, from inviscid to viscous laminar flows, from subsonic to supersonic flows.

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An Arbitrary Lagrangian-Eulerian Algorithm for Multiphase non-Newtonian Fluid Flows

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Key Words: non-Newtonian, Multiphase Flow, Arbitrary Lagrangian-Eulerian, Rising Bubble, Mass Conservation

Multiphase non-Newtonian flows are encountered in nature (e.g., particle-laden biological flows) and industrial applications (e.g., ink jet plotter). Numerical simulation of multiphase non-Newtonian flows is quite challenging because of the discontinuous material properties across the surface, a priori unknown deforming interface location, large extra stress values and large difference between polymer relaxation time and advective time scale (i.e., high Weissenberg number problem). In this study, the Arbitrary Lagrangian Eulerian (ALE) approach [1, 2] is extended to isothermal non-Newtonian fluids by implementing constitution equations. To the best of our knowledge, the ALE algorithm based on the side-centered unstructured finite volume method has been applied to the simulation of non-Newtonian multiphase fluid flows for the first time. The pressure field is treated to be discontinuous across the interface with the discontinuous treatment of density and viscosity. The discontinuous treatment of pressure field helps us to avoid errors due to the incompressibility condition in the vicinity of the interface. The surface tension term at the interface is treated as a tangent force. The jump conditions are exactly satisfied across the interface. The parasitic currents are found to be very sensitive to the computation of normal vectors [2]. Therefore, the mean weighted by sine and edge length reciprocals (MWSELR) is implemented for the computation of unit normal vector. The resulting algebraic equations are solved in a fully coupled (monolithic) manner and an approximate matrix factorization similar to that of the projection method is employed. The parallel algebraic multigrid solver BoomerAMG provided by the HYPRE library, which is accessed through the PETSc library, has been utilized for the scaled discrete Laplacian of pressure and the diagonal blocks of mesh deformation equations. The classical benchmark problem of a single rising Newtonian bubble in a non-Newtonian fluid due to buoyancy is presented in two- and three-dimensions.

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Computational Analysis of Shear-thinning Coating flows

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Key Words: *Shear-rate-dependent viscosity, Industrial applications, Mircrovortices, Pulsatile flows*

Complex fluids with shear-rate-dependent viscosity are widely used in the flows of several industrial applications. To have better control of the flows of such fluids, it is crucial to understand the underlying principles that govern the fluid flow. In this study, through two illustrative case studies, we present the use of flow modeling and simulation for a better understanding of the effects of shear-rate-dependent viscosities on the fluid flow.

In the first case, we explore the effect of the shear-rate-viscosity on the operating conditions that lead to the formation of microvortices in the slot coating flows, which are known to have a detrimental effect on the stable process operation and production of defect-free film products [1]. We simplify the microvortices found in the downstream region of slot coating flow as flow reversal and present the effect of the shear-rate-dependent viscosity on the critical operating conditions at the onset of the flow reversal [2].

Two methods for computing the critical condition in slot coating flows of generalized Newtonian fluids (GNFs) are presented. The two methods were applied to the flows of two illustrative GNFs, the Carreau-Yasuda, and Bingham-Carreau-Yasuda fluids. They were both found to be successful in computing the critical flow reversal conditions. It was also revealed that the critical conditions depended significantly on the local power-law index n, which quantifies the dependency of the viscosity on the magnitude of the shear rate.

In the second case, we explore the flow properties of pulsatile shear-thinning flows in a two-dimensional rectangular channel [3]. Since various external disturbances such as oscillations from flow pumps are commonly encountered in industrial processes and such disturbances may result in unexpected changes of the rheological properties of the complex fluids.

The characteristic viscosity chosen based on the steady-state analysis was defined for the pulsatile shear-thinning flow. It was used to form a non-Newtonian Womersley number, which acts as a critical model parameter of the system of interest. Numerical analyses of Carreau fluids revealed the existence of master curves for the amplitudes and phase lags of the flows. We advanced further to demonstrate that the flow dynamics can be predicted using the pre-computed master curves with high accuracy without explicit transient computations.

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Computational models and experimental studies of mold filling in thin channels with yield stress fluids

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Key Words: *Mold filling, yield stress, viscoelastic, Saramito model, finite element, moving mesh*

Materials that behave as both fluids and solids can be seen in a wide variety of applications from pouring concrete to lava flows and food processing. Yield stress is a useful concept for developing models that demonstrate both fluid and solid behavior depending on the local state of the fluid. In this talk, we will discuss an ongoing project to use elastoviscoplastic models to understand the complex flow profiles of a model yield stress fluid, Carbopol, as it evolves in time in a free surface flow. We use a Saramito model to describe the rheology of the fluid [1]. This model describes the material as a Maxwell fluid above yield and an elastic solid below yield, with a yield criterion based on the von Mises stress. Conservation equations for momentum and mass and the Saramito constitutive equations for stress are solved using the finite element method coupled to a free-surface moving mesh algorithm. We verify our implementation by comparing our results to benchmarks in the literature such as flow past a sphere and a ball falling in a tube full of yield stress fluid. Furthermore, we compare results from mold filling simulations to validation flow visualization experiments in a quasi-two-dimensional flow where fluid fills a thin gap between transparent plates. The experiments show regions of low strain where the fluid displaces as a solid body and high strain regions where the Carbopol is fluidized. The computational model matches qualitatively for the yield stress fluid. Comparisons between the quasi-two-dimensional model and the fully three-dimensional will also be discussed.

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Efficient glow discharge solver for sensitivity analysis

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Key Words: plasma kinetics, glow discharge, Chebyshev collocation method, time periodic shooting

This talk aims to highlight the development of an efficient solver for the capacitively coupled glow discharge device within the scope of sensitivity analysis. The physical model is comprised of species continuity equations, electron and heavy species energy equations, and Gauss' law, closed by the drift-diffusion model and a chemical reaction mechanism, driven by an oscillating voltage applied on one side of the domain [1]. The high-aspect-ratio parallel-plate glow discharge device lends itself to a 1D analysis, meaning the model consists of a set of 1D, unsteady PDEs, where the solution of interest is periodic in time. The large number of simulations required for sensitivity analysis and UQ implies the need for a solver that rapidly converges to the periodic steady-state solution. However, the very slow ambipolar diffusion processes in a capacitive glow discharge, especially for pressures in the Torr regime and higher, means it can take thousands of periods of forward simulation to approach this periodic solution. To speed up this convergence, we have implemented a time-periodic shooting (TPS) algorithm [2], in which the periodicity of the solution is imposed as an additional constraint, and the resulting nonlinear system is solved using a standard Newton method. This approach is observed to be 100 times faster than time marching alone, which has enabled an initial global sensitivity analysis. Specifically, we have conducted an initial study using the libraries Chaospy [3] and Uncertainpy [4], in combination with the TPS-based glow discharge solver, to determine which input parameters (i.e., reaction rate coefficients and transport parameters) most influence the quantities of interest, e.g., electron density.

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Novel Space-Time Finite Elements for Fluid-Based Processes

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Key Words: Deforming Domains, Space-Time Finite Elements

Moving-boundary flow simulations are an important design and analysis tool in many areas, including civil and biomedical engineering, as well as production engineering. Interface-capturing offers flexibility for complex free-surface motion, while interface-tracking is very attractive due to its mass conservation properties at low resolution. We focus on these alternatives in the context of flow simulations based on stabilized finite element discretizations of Navier-Stokes equations, including space-time formulations that allow extra flexibility concerning grid design at the interface.

Space-time approaches offer some not-yet-fully-exploited advantages; among them, the potential to allow some degree of unstructured space-time meshing. A method for generating simplex space-time meshes has been developed, allowing arbitrary temporal refinement in selected portions of space-time slabs. The method increases the flexibility of space-time discretizations, even in the absence of dedicated space-time mesh generation tools. The resulting tetrahedral and pentatope meshes are being used in the context of cavity filling flow simulations, such as those necessary to design injection molding processes.

In cases where a general space-time mesh is still out of reach, a variety of special approaches involving slipping and deactivation of elements can be used. Several examples will be given.

This is a joint work with Violeta Karyofylli, Max von Danwitz, Norbert Hosters, Michel Make, and Linda Gesenhues.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Numerical simulation of polymeric mixing process with non-conforming methods in OpenFOAM

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Key Words: Non-conforming methods, Non-Newtonian fluids, Polymeric mixing

Mixing of polymeric materials is performed with the aid of machines characterized by complex geometries in which body-fitted simulations can hardly be applied. The adoption of non-conforming approach (such as diffuse interface, ficticious domain, immersed boundary or volume penalty methods) represent valid alternatives to simulate such processes with complex kinematics (single and twin screw extruders, banbury mixers etc.).

In this talk we present the results of a research activity finalized to the development of a simulation tool based on the open-source CFD library OpenFOAM for the analysis and optimization of the mixing process of polymeric materials. Different non-conforming discretization strategies, namely a diffuse interface penalisation method [2] and a discrete-forcing direct-imposition immersed boundary method [1], and different solution strategies for the solution of non-Newtonian fluid flows with temperature dependent viscosity are compared in terms of accuracy, robustness and computational cost.

Numerical results for simple similar industrial geometries and flow conditions will be presented and discussed.

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RANS Model Assessment for Curved Turbulent Shear Layers and Retro-propulsive Flows

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Key Words: RANS modelling, compressibility effects, curvature effects, retropropulsion

Solving the Reynolds-Averaged Navier-Stokes (RANS) equations is one of the most affordable methods in CFD and remains vital in vehicle design and analysis. However, RANS solvers' deficiencies in capturing complex flow fields, such as those in supersonic retro-propulsive (SRP) flows, are well acknowledged [2, 5]. This work addresses the challenge of characterizing turbulence in retro-propulsive jet plumes by direct comparison of high-resolution large eddy simulations (LES) and RANS, to assess and improve turbulence modeling in canonical elements of SRP flows. The first component of this study is the production and analysis of LES of curved turbulent shear layers with varying compressibility, density variation, and curvature intensity using NASA's OVERFLOW code [3]. The second component of this study will focus on three of the most popular RANS models – the Spalart-Allmaras model, the $k-\omega$ model, and Menter's shear stress transport model. These high-fidelity studies enable an understanding of turbulent mixing characteristics when influenced by multiple competing physical mechanisms. RANS model comparisons with the LES database will demonstrate the state of the art in RANS models for these complex flows and highlight areas for improvement. In addition to the standard models, the performance of several turbulence model corrections will also be considered. Among others, Suzen & Hoffman's compressibility correction [4], which was formulated to assist the behavior of compressible free shear flows and targets the $k-\varepsilon$ part of Menter's models, and Catris & Aupoix's density gradient correction [1] are considered in this work. Preliminary comparisons of RANS and LES data suggests that the present RANS models with standard model coefficients show significant bias error relative to LES data in regards to mixing layer growth rates. This is a collaborative study with Dr. Robert Childs at NASA Ames Research Center.

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Simulation of a droplet impact in a thin film using a phase-field model

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Key Words: Two-phase flow, Phase-Field method, Drop impact

Droplet impact dynamics are an active research area due to the variety of their industrial applications. It appears in industrial processes employing spray coating and painting, spray cooling, inkjet printing, combustion engines, and anti-icing characteristics of critical industrial components such as aircraft surface, powder lines, and wind turbines [1]. The droplet impact is a special case of two-phase flow simulations, where the surface tension force plays an important role. One way to model the gas and fluid phases is with interface capturing methods. Three well-established interface capturing models are the Volume-of-Fluid (VOF), level-set, and phase-field models [2]. The main advantage of the VOF method is mass conservation, while the implementation of the surface tension may be challenging. The level-set is known for its ability to compute the surface tension accurately, and phase-field models are known for satisfying the second law of thermodynamics. This work uses a conservative Allen-Cahn equation based on [3] to model and simulates a liquid drop impact on a moving wall with a pre-existing thin film of the same liquid. We couple this interface-capturing method with the Navier-Stokes equations. The analysis takes into account viscous, inertial, and surface tension forces, neglecting gravity. We solve the equations with the residual-based variational multiscale finite element formulation. We implement the whole model in `libMesh`, an open finite element library that provides a framework for multiphysics, considering adaptive mesh refinement. The values of the Reynolds and Weber numbers determine different drop splash regimes. Numerical results are presented for 2D and 3D liquid drop impacts, and they are in good agreement with other simulations.

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Validation of Laminar Stirred Mixing CFD Models using Positron Emission Particle Tracking

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Key Words: *Computational Fluid Dynamic (CFD), Positron Emission Particle Tracking (PEPT), laminar flow stirred mixing, model validation*

Industrial fluid mixing is a unit operation intrinsic to the production of many Fast-Moving Consumer Goods (FMCG). Because there is a lack of analytical techniques capable of predicting the hydrodynamic flow of complex rheologies, the current challenge in these industries is how best to optimise the mixing of these fluids [1].

The research presented will focus on the development of Computational Fluid Dynamics (CFD) models capable of predicting mixing for rheologically complex systems in the laminar flow regime for a horizontal bladed mixer, reducing the need for costly experimental trials. The general method of model development is to build on simple Newtonian models by validating each iteration with experiment and to gradually add elements of complexity such as a non-Newtonian rheology. The main method of validation is Positron Emission Particle Tracking (PEPT), a powerful technique reliant on ergodicity which can generate a Lagrangian description of hydrodynamic flow *in-situ*. PEPT uses gamma-ray detectors to locate tracer particles in transit and is used uninvasively in opaque industrial equipment [2]. Validation using PEPT entails a 3D pointwise comparison of multiple parameters predicted by the CFD model containing multiple closure relations.

The current CFD model is developed in Siemens STAR-CCM+ and uses an Eulerian sliding mesh with a Volume of Fluid (VOF) physical model. With iterative validation, the next stage of the model is to predict the behaviour of the PEPT tracer particle by incorporating the Discrete Element Method (DEM) to ultimately create validated CFD-DEM models that can predict the coupled properties for a variety of rheologically complex laminar mixing systems.

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Geometry Influence of Particles Depositing in Realistic Human Lung Replicas

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Key Words: *OpenFOAM*, *Air Pollutants*, *Human Airways*, *Particle Deposition*, *Superellipsoids*

Humans are constantly exposed to pollutants in the air. These particles can originate from pollen, tyre wear, exhaust residue, microplastics, fabrics as well as asbestos fibres or, as highlighted in the recent pandemic, expiratory events leading to exhaled viruses encapsulated in saliva droplets. Understanding particle deposition in the human lung is of key interest to reduce the impact of harmful particles, or on the contrary, to improve the targeted delivery of drugs to reduce their side effects. A common simplification in the study of particle deposition in human airways is to assume perfectly spherical particles. This is an accepted approach for studies of aerosolized droplets, yet for inhalation of toxic fibres or arbitrarily shaped aerosol particles such as pollens, fibers or volcanic ash, the assumption of spherical shape no longer applies. In this context, shape factors are often used to account for non-sphericity effects, but these are often insufficient to accurately predict particle motion. Therefore, more sophisticated particle models need to be considered. However, there is a glaring lack of research in this area regarding the accurate prediction of inhalation of more complex shaped particles in realistic human airways. In this work, we investigate the effect of different particle geometries on the deposition behaviour in realistic lung models. The study includes spheres and prolate ellipsoids as well as more arbitrary shapes in the scope of superellipsoidal particles, fitted to naturally occurring pollutants, to cover a wide range of particles suspended in the air we breathe. In our study we focus on the deposition efficiency in the mouth-throat and tracheobronchial region as well as the level of bifurcuration of the chosen lung geometry. The computational study is based on Lagrangian particle tracking in RANS resolved turbulent flow in a realistic lung geometry performed using an in-house solver developed in the OpenFOAM framework. Finally, we present the identified key influences on deposition efficiency in the lung models used.

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Numerical Analysis of Interaction between Multiphase Flow and Rain Chain

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Key Words: *Multiphase flow, Motion of connected bodies, Cartesian grids, Level-set method, Immersed boundary method*

A numerical analysis of the motion of a rain chain in multiphase flow was performed. The rain chain was modeled using connected cups. This study primarily discussed the relationship between the motion of the rain chain and the flow of running water from the top of the chain. The incompressible continuity and the Navier–Stokes equation were solved by means of the finite difference method on a staggered Cartesian grid. The velocity–pressure coupling was solved using the fractional step method. The interface between the two fluids was defined by means of the coupled level set and volume of fluid method [1]. In the Cartesian grid, the moving body was modeled using the body force-type immersed boundary method [2]. The surface tension was modeled by the continuum surface force model [3]. It was shown that the motion of the rain chain changes greatly depending on the conditions of the running water, the mass of the cups of the rain chain, and the number of the connected cups. In the case of a rain chain that comprised 10 cups, the displacement of the motion gradually increased and twisting motion was observed.

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Numerical Investigation of Rising Bubbly Flows in Slightly Inclined Vertical Pipe Filled with Power-law Fluid

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Key Words: *Bubbly flow, Bubble Dynamics, Inclined Pipe, Lateral Motion, Negative Buoyancy Effect.*

Three-dimensional direct numerical simulations are conducted for bubbly flows rising in a slightly inclined vertical pipe using the method developed by Ii et al. [1]. In the present method, multiple VOF function is introduced to avoid bubble coalescences and 78 rising bubbles are solved without coalescence which are often observed in the actual flows with contaminant effect. The simulation results are validated through the comparisons with the previous experimental data by Zenit et al. [2] for the inclined angle of 5 degree. The simulation results showed the good agreement with their experimental data. For other conditions, we have found interesting phenomena for lower inclined angle. The results show a negative buoyancy effect. That is, when the inclined angle is small enough (< 2 degrees), bubbles shown the lateral migration in the pipe against the buoyancy effect. This negative buoyancy effect disappears when the inclined angle becomes bigger than 2 degrees. To investigate the mechanism of negative buoyancy effect, we conducted the analysis of the force acting on a bubble. Due to the dynamical motion of a rising bubble, it is difficult to get the force by simply integrating the stress on bubble surface. Here, we introduce the macroscopic control volume analysis using the control volume containing an individual bubble inside. The analysis show that the negative lift force is caused by the unsteady component of the liquid phase.

We also conducted the simulations for non-Newtonian, Power-law fluid. The effect of power index and flow consistency index are investigated. The obtained results can be related to some practical applications such as deep ocean mining using an air-lift pump [3].

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Numerical Simulations of Hydrogen Production in Alkaline Water Electrolysers

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Key Words: *Multiphase flows, Bubbly flows, Electrochemistry, Industrial Applications, Multiphysics Problems*

Alkaline water electrolysers are commonly used for the industrial-scale production of hydrogen. Operating at high current densities leads to enhanced hydrogen production but reduced cell efficiency, partly due to ohmic losses from the gas-liquid flow. Gas blockage of the electrode surface and reduced effective electrolyte conductivity from increased void fraction are key contributors to these losses. We perform three-dimensional transient numerical simulations of an electrochemical cell under galvanostatic conditions, modelling the multiphase flow and the electrochemistry with the OpenFOAM libraries. We use a multifluid Eulerian model to simulate the bubbly flow, with oxygen and hydrogen as dispersed phases and the electrolyte solution as the continuous phase. The current distribution in the electrolyte is coupled to the Butler-Volmer equation at the electrode surfaces, and governs the local gas generation rate through Faraday's law. We investigate both free convection [1] and forced convection [2] configurations over a range of current densities, and compare void fractions, velocity profiles, turbulent intensity and cell potential with experimental results to validate our model. We then explore the impact of bubble size, distribution and inter-phase coupling terms on the flow in the cell, and observe the formation of waves along the electrode surface. We study the phenomena which give rise to these waves, and their impact on cell operation. Improved modelling and understanding of the flow within alkaline water electrolysers paves the way for optimisation of cell design and operation from a fluid mechanics perspective.

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Pore-Scale Mechanisms Control Fluid Invasion during Multiphase Flow in Regular Porous Media

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Key Words: *Porous Media, Multiphase Flow, Fluid Displacement*

The unstable fluid-fluid displacement patterns in porous media, featured with rough invasion fronts and trapping of the defending phase, are often observed in drainage processes, i.e., when the porous media are non-wetting to the invading phase. On the contrary, during imbibition, faceted and compact growth is expected in porous media with geometrically homogeneous pore structures. This is because the pore-scale non-local cooperative pore-filling event is favoured. In this work, we report the irregular growth of the invading fluid during imbibition processes in two-dimensional regular porous media composed of circular posts arranged on triangular and square lattices. The ramified invasion patterns associated with thin fingers and trapping of the defending fluids are reminiscent of capillary fingering, which are often observed only in drainage condition. Through examining the capillary pressure signals and type of pore-scale invasion mechanisms during multiphase flow, the differences between compact and faceted displacement and unstable growth are revealed. The critical events at pore-scale that determines the pore-filling process are analysed, leading to a phase diagram describing the dominance of event type across a wide range of porosity and wetting condition. Through conducting systematic quasi-static radial injection simulations, excellent agreement is observed on the transition boundary from faceted and compact displacement patterns towards irregular and dendritic invasion morphologies. This is reflected by the overlap of the transition boundaries from analytical prediction, type of pore-scale invasion events, and macroscopic morphology quantified by the fractal dimension. This work provides new insights on the role of geometrical features of solid structures during fluid displacement process with emphasis on the porosity and wettability of regular porous media. The findings would assist in guiding the design of microfluidic devices to deterministically control the multiphase flow, transport and reaction processes.

The influence of flow conditions on mass transfer in lyophilization in a vial

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Key Words: *Lyophilization, Heat and Mass Transfer, Computational Fluid Dynamics, Vial*

Modeling lyophilization in a vial is frequently done on a single vial level. When setting up the numerical model, the main focus is on the heat and mass transfer inside the lyophilizate, whereas the vapor dynamics in the upper part of the vial is taken into account simply through imposing the system pressure as a pressure boundary condition. The present research offers a deeper insight into the interaction of sublimated vapor flow and vial internal geometry by performing a detailed CFD analysis of the flow field inside and in the vicinity of a vial with installed stopper. The main attention is devoted to the analysis of the corresponding vapor pressure conditions inside the vial and their influence on sublimation kinetics, which governs the process inside the lyophilizate and which is modeled by a dedicated 0D lyophilization model. The derived computational model is based on a coupled numerical solution of the heat and mass transfer inside the lyophilizate by means of a 0D vial lyophilisation model and the 3D fluid flow through the vial. Due to low system pressures, the slip flow regime is considered, leading to the need of imposing the velocity slip conditions at the vial walls. The coupled model results in terms of temperature at the lyophilizate bottom and mass flow rate are validated with the results of dedicated experiments on the laboratory scale lyophilizer and Schott R6 vials, with 20mm internal and 13 mm throat diameters, respectively. The computational study shows that the vial geometry, especially the installed stopper, alters the pressure field conditions inside the vial, which results in a decrease of numerically computed mass flow rate and an increase of computed sublimation front temperature. The effect is more pronounced in the case of lower system pressure settings (typically 5 – 10 Pa), and can result in up to 4.5% difference in the computed primary drying times and up to 2K higher resulting bottom temperatures compared to the results of 0D model without considering the influence of the vial geometry. The obtained results show that the coupled numerical model can be successfully used in studies of the impact of various vial forms as well as stoppers on the lyophilization kinetics in a vial.

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Estimation of the state of matter in young impact craters on the Moon based on the orbital observations

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Key Words: *Lunar matter, Impact craters, Orbital observations, State of matter, Estimation of state, Crater structure, Forthcoming expeditions, Applied and fundamental aspects*

The report examines the results of a 3D-survey of the relief in young impact craters based on high-resolution images obtained from lunar orbits. The craters examined included: the Tsiolkovsky and Aitken craters on the far side of the Moon, the Tycho and Ina craters of the visible hemisphere, as well as the Orientale Mare in the marginal zone of the Moon. To build 3D-models, orbital images of the Soviet spacecrafts "Zond-6,-8" and the American spacecraft "Apollo-17" delivered to Earth, as well as images transmitted to Earth from the Lunar Reconnaissance Orbiter (LRO) were used.

The survey of the relief using 3D-models allows us to study the structure of craters from different sides at different angles of view at different scales. This approach, in addition to analyzing single images, opens up new possibilities. In particular, on a 3D-model, it is often possible to detect relief details that are either not visible in single images, or are not clearly visible enough. So, looking through the images from the “Apollo-17” spacecraft, made on different orbit revolutions at different positions of the Sun, which provided different illumination conditions, we found a small volcano on the floor of the Tsiolkovsky crater, surrounded by an oval-shaped depression of soil about 25 km in size [1], which no one had paid attention to before. Further study of the object we found allowed the authors of the work to make an assumption about the presence of a magma chamber under the bottom of the crater. Another example of this approach is associated with the Aitken crater. Comparing our 3D-models of the central peak of Aitken crater with ultra-high resolution images from the LRO, we found a glacier-like tongue crawling out directly from the southwestern slope of the central peak to the crater floor [2]. It was possible for the first time to examine its structure and find similarities with similar objects on Mars. The report provides a detailed analysis of all 5 the above-mentioned objects.

Forthcoming lunar expeditions, creation of lunar bases and mining of minerals presupposes a certain level of knowledge about the lunar surface itself. The state of the matter of lunar craters, the structure of the elements of the lunar relief and the lunar interior is of particular interest in this regard. The results obtained play an essential role in understanding the crater formation process itself, as well as for studying the physics of the extreme state of matter. It is also important to note that the energy of crater-forming events is so high that it is unlikely that it will ever be possible to reproduce it in terrestrial conditions.

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Transport of logarithmic potentials versus process duration

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Key Words: *Transport*, *Dynamical Equilibrium, Logarithmic Potentials, Measurements*

Transport phenomena allow us the possibility of understanding and modeling many of the multi-scale dynamics problems of natural sciences and engineering. Particularly, in this work we transport logarithmic potentials such that its parameters are measured in order to match the dynamical balance in a context of a multiplicity of interacting forces where all can be derived from Bayesian theories in close connection with statistical meanings and actual applications. In this scenario, the Gamma function emerges lightly changed from its classical form and plays an important game allowing the time estimation of a process associated to many dynamical models. Although, the Gamma function is associated with a wide variety of applications related to natural numbers, solutions of variable coefficients differential equations, power series, integrals and much more issues in the literature for instance [1-6], this work focuses specifically on the estimation of time of duration in dynamic processes. These processes are possible in scientific experiments but also in the current life, the one people live day by day, at any scale, at any time, period or epoch. So then, three different situations are considered. First, we obtain a non-classical and not common property of the Laplace Transform, in the context of Transport equations and logarithmic potentials. Second, the Gamma function emerges as a balancing solution and it does in an apparently new generic form, so it is worthy to be presented. Third, a formulation for the duration time of a process is provided when we truly predict that the end of the process is reached, successfully. On the other way, some comments related to when we should not wait anymore the end of one process, are given. Hypothetically, this is because from the theoretical approach we should be able to know whether the end of the process will never come. Finally, some related facts are discussed.

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Detailed simulations of nozzle-dependent primary atomization in coaxial atomizers

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Key Words: Coaxial Atomizer, Primary Atomization, Nozzle Internal Flow, Volume of Fluid

Coaxial atomizers are widely used in industrial spray applications, and it is well known that their high-speed gas flow features, determined by the nozzle geometry, are crucial for the breakup process [1]. As such nozzles often include complex geometry features like sharp edges, computational strategies for simulating primary atomization need to capture the details of the nozzle internal flow. This results in a challenging multiscale problem for computational strategies.
In this work, a simulation approach for detailed simulations of nozzle-dependent primary atomization for a coaxial atomizer is presented. To address the multiscale nature, a one-way coupling approach is used, which divides the entire simulation domain into a single-phase nozzle internal flow simulation domain and primary breakup simulation domain. Coupling between both domains is achieved by imposing the unsteady velocity field at the nozzle outlet plane as inlet conditions for the interface resolving primary breakup simulation. The nozzle internal flow is computed in a large-eddy simulation using the low-Mach solver of the in-house code CIAO. The interface resolving primary breakup simulation is computed as direct numerical simulation with a recently developed 2^{nd}-order conservative unsplit Volume of Fluid method [2], which is coupled to a sharp-interface flow solver [3].
The simulation approach is applied to the coaxial atomizer of the SpraySyn burner and an additional complex nozzle geometry that has been studied in the same context [4]. Both simulations share the same nominal non-dimensional parameters, which allows evaluating the impact of the nozzle geometry on primary breakup. The results show that the simulation approach can capture nozzle-dependent atomization, and the observed qualitative and quantitative results are discussed in the context of the nozzle internal flow features.

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Dynamics and Modelling of Spin-affected Droplet Collision

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Key Words: *Droplet collision, Volume of Fluid method, spinning droplet, bouncing, separation*

Droplet collision is closely related to many spray processes in nature and industry, and it has been extensively studied and reviewed[1] in the literature. Modelling of droplet collision is significant for the Eulerian–Lagrangian spray simulation[2]. The Volume-of-Fluid (VOF) method[3] serves as an efficient analysis tools to study the physics and modelling of droplet collision [4, 5].

By far, almost all studies on droplet collision were focused on initially non-spinning droplets. However, in practical situations of dense sprays, the dispersed droplets usually have spinning motions and are highly likely to collide with each other. The spinning motion can be created either from the preceding off-center collisions (owing to the nonzero total angular momentum) or the non-axisymmetric breakup of impinging jets. Droplet spinning motion was neglected in the previous experimental studies probably because it is technically challenging to generate stable spinning droplet and quantitatively characterize the spin velocity. However, it is relatively easy to set up the spinning droplet in a VOF simulation.

In the present study, the significance of droplet spinning motion is numerically verified by quantitatively characterizing the trajectory of mass center and spinning speed of colliding droplets. Then, the relevant canonical phenomena, such as coalescence, bouncing, and separation between spinning droplets, are simulated. For droplet coalescence, a prominent discovery is that the spinning droplet can induce significant nonaxisymmetric flow features and substantially promote the mass interminglement of droplets. For droplet bouncing, a practical modelling of momentum recovery coefficient in determining the post-collision velocities is proposed based on the interchange between the orbital angular momentum and the spin angular momentum during droplet collision. For droplet separation, a unified model of droplet separation (reflexive and stretching separation) was established to analyse the effect of droplet spin chirality on boundary transition. These results enhance our understanding of the dynamics and modelling of droplet collision.

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Electric-Field-Driven Ion Emission from the Free Surface of Room Temperature Ionic Liquids

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Key Words: *Electrospray, Ionic liquids, Ion emission, Molecular simulation*

Electric-field-driven ion emission from the free surface of a planar room-temperature ionic liquid (RTIL) film was studied by using molecular dynamics simulations. We calculated ion emission rate (j_e) as a function of the electric field normal to the RTIL/vacuum surface (E_n) and found that the logarithm of j_e over the charge density on the surface (σ) is proportional to $E_n^{1/2}$, in agreement with classical ion evaporation theories. The composition of emitted ions includes monomers and dimers. It was found that the monomer has to move across two barriers before emission. The fraction of dimers was found to depend on the external field and ion-ion interactions. We further performed replica exchange molecular dynamics simulations and identified different metastable states of the emitting ion near the liquid film. Our results showed that E_n and molecular details of ion/surface determine the rate and composition of ion emission from RTIL/vacuum surfaces. Fundamental insights revealed in this study form the basis to improve ion evaporation theories and performance of electrospray applications ranging from space propulsion to nanomanufacturing.

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Experimental investigation on the spreading progress after droplets impacting on to a vertical vibrating plate at low frequency

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Key Words: *Drop impact, Vibration, Weber number, Spreading, Rim, Inner lamella*

The impingement of fuel droplets on the piston surface would greatly affect the combustion process and emission generation of direct injection diesel engines. In this paper, to mimic the interaction between the droplets and vibrating engine body, the dynamic behaviors of droplets impacting on a vertically vibrating plate were explored experimentally. The main target of this paper is the spreading process from the droplet attaching the plate to it reaching the maximum diameter. Several groups of impacting heights and plate vibrating frequencies were set to obtain a broad range of Weber numbers. The temporal evolutions of the inner lamella and rim after impact were traced by high-speed photography. The results show that the maximum spread time of the inner lamella maintains a relatively stable value, and the whole spreading time depend on the growth time of the rim. The fluctuation range of the growth time of the rim increases under increased vibrating frequency, while decreases with the increase of impacting height. The fluctuation range of the thickness of rim would be smaller with higher impacting height, and the relationship between growth time of rim and impact phase is sinusoidal at the same impacting height and frequency. The existence of air forces plays a key role in the development of the liquid layer. In addition, the maximum spread radius would be smaller for droplets with an impacting height of 15 cm, because the ring-shaped rim would receive more resistance from viscous forces and surface tension than fingers. Finally, an empirical formula based on Srivastava's model was built to accurately predict the maximum spread factor of droplets after impacting on the vibrating plate, in which the influence of the impact phase, vibration frequency and Weber number were incorporated.

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Front-Tracking approaches for the modelling of breakup and coalescence

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Key Words: Two-phase flows, Front-Tracking, Breakup, Coalescence, Multi-scale

In this work two-phase flows are modelled by a multi-scale approach involving dedicated meshes, one for the interface, mobile and deformable, for the Front-Tracking [1] and called Lagrangian, and the other Eulerian and fixed for the conservation equations of mass and momentum.

These multi-scale models are difficult to achieve numerically because they require managing dynamically in time and space the mesh of the interface (made up of connected triangles). In exchange for this complexity, they offer an explicit description of the interface even in the presence of strong curvatures and a better control of topological changes (coalescence and breakup). The models and algorithms must run in parallel on distributed memory computers to conduct convergence studies, validate academic cases and then tackle more complex configurations.

In order to describe efficiently the thin features of the interface, we implemented an adaptive remeshing procedure with local surface reconstruction. Topological changes are handled geometrically. The volume fraction is calculated with a geometric method: the Ray-Casting with local refinement.

Experimental and numerical configurations from the literature will be used to verify the models and numerical methods. Among them, we can mention the collision of two drops [2].

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Fully Compressible Numerical Simulations of Primary Breakup Processes in Dual Fuel Internal Combustion Engines

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Key Words: *Fully compressible flow; implicit large eddy simulation; duel fuel internal combustion engine; primary breakup; diffuse interface method; continuum surface force model*

Carbon neutrality is imminent and Dual-fuel Internal Combustion Engines (DFICE) using fuel mixtures have the potential to meet stringent emissions regulations. However, there are only few high-resolution studies on the primary breakup process under DFICE conditions. In this work, we develop a numerical algorithm capable of handling DFICE primary break-up and compressibility of all involved phases including surface tension effects. An Implicit Large Eddy Simulation (ILES) approach for compact stencils proposed by Egerer et al. [1] is used, which is based on the Adaptive Local Deconvolution Method (ALDM) by Adams et al. [2] and Hickel et al. [3]. ILES merges sub-grid turbulence with the numerical truncation properties of the scheme. We apply a diffuse interface method (DIM) together with an improved barotropic multi-component fluid model, and a continuum surface force (CSF) model [4] with algebraic interface sharpening treatment, which have recently implemented into our code CATUM. Results from the "recovery from square bubble" case and further standard cases are in very good agreement with reference solutions. A discontinuity sensor switches the cell-face value reconstruction procedure between an upwind-biased and a centered reconstruction scheme, along with proper limiters. Time integration is performed by an explicit, four-stage Runge-Kutta method.

We investigate two different n-dodecane mass flow rates for the "Spray A-210675 model" with an initial pressure of 6MPa and a mixture of 80% Nitrogen and 20% Methane in the chamber. The computational domain is 10D*10D*20D. The computational grid with a smallest mesh size of 0.04μm is applied and the obtained results are analyzed in detail. At high mass flow rate, in-nozzle instabilities and Kelvin-Helmholtz instabilities dominate the primary breakup independent of the surface tension. The disturbance generated by the head of the mushroom jet transmits through the gas mixture to the upstream liquid area and causes the instability to grow in the direction of the liquid core. In case of a low mass flow rate, Rayleigh instabilities become relevant. The results improve our knowledge on how these instabilities develop and contribute into DFICE atomization, providing data on effective designs of DFICE components including Fuel Injection Equipment (FIE) and providing reference data for DFICE primary breakup processes, as detailed experimental measurements and visualizations are insufficiently available.

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Influence of Density and Viscosity on Deformation, Breakage and Coalescence of Bubbles in Turbulence

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Key Words: Bubbles, Bubbles Deformation, Breakage and Coalescence, Density Ratio, Viscosity Ratio

We investigate numerically the effect of density and viscosity differences on a swarm of large and deformable bubbles dispersed in a turbulent channel flow. For a given shear Reynolds number, $Re_\tau = 300$, and a constant bubble volume fraction, $\Phi \simeq 5.4\%$, we perform a campaign of direct numerical simulations (DNS) of turbulence coupled with a phase-field method (PFM) accounting for interfacial phenomena. For each simulation, we vary the Weber number (We, ratio of inertial to surface tension forces), the density ratio (ρ_r, ratio of bubble density to carrier flow density) and the viscosity ratio (η_r, ratio of bubble viscosity to carrier flow viscosity). Specifically, we consider two Weber numbers, $We = 1.50$ and $We = 3.00$, four density ratios, from $\rho_r = 1$ down to $\rho_r = 0.001$ and five viscosity ratios from $\eta_r = 0.01$ up to $\eta_r = 100$. Our results show that density differences have a negligible effect on breakage and coalescence phenomena, while a much stronger effect is observed when changing the viscosity of the two phases. Increasing the bubble viscosity with respect to the carrier fluid viscosity damps turbulence fluctuations, makes the bubble more rigid and strongly prevents large deformations, thus reducing the number of breakage events. Local deformations of the interface, on the contrary, depend on both density and viscosity ratios: as the bubble density is increased, a larger number of small-scale deformations, small dimples and bumps, appear at the interface of the bubble. The opposite effect is observed for increasing bubble viscosities: the interface of the bubbles become smoother. We report that these effects are mostly visible for larger Weber numbers, where surface forces are weaker. Finally, we characterize the flow inside the bubbles; as the bubble density is increased, we observe, as expected, an increase in the turbulent kinetic energy (TKE) inside the bubble, while as the bubble viscosity is increased, we observe a mild reduction of the TKE inside the bubble and a strong suppression of turbulence.

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Manifold death: the implementation of controlled topological changes in thin sheets by the signature method

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Key Words: Two-phase flows, Volume of Fluid, Breakup, Topology changes

A well-known drawback of the Volume-of-Fluid (VOF) method is that the breakup of thin liquid films or filaments is mainly caused by numerical aspects rather than by physical ones. The rupture of thin films occurs when their thickness reaches the order of the grid size and by refining the grid the breakup events are delayed. When thin filaments rupture, many droplets are generated due to the mass conserving properties of VOF. Thus, the numerical character of the breakup does not allow to obtain the desired convergence of the droplet size distribution under grid refinement. In this work, we present a novel algorithm to detect and perforate thin structures. First, thin films or ligaments are identified by taking quadratic moments of the VOF indicator function. Then, the breakup is induced by making holes in the films before their thickness reaches the grid size. We show that the method improves the convergence upon grid refinement of the droplets size distribution, as well as of enstrophy.

Modeling of Two-Phase Vapor-Liquid Spray with Flash Boiling

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Key Words: *Flash Boiling Spray, Phase Change, Speed of sound, Internal Combustion Engine*

ABSTRACT

In internal combustion engines such as diesel and gasoline engines, Flash boiling phenomenon of fuel spray has a significant effect on the liquid atomization process and the mixture formation process. There are many experimental reports on the phase change process in spray formation with flash boiling, however, the phenomena remains unclear and quantitative prediction of the phenomena is difficult. Flash boiling is a phase change process from liquid to vapor that occurs when the pressure drops below the saturated vapor pressure of the liquid caused by a sudden pressure change. In the nozzle, the rapid phase change is due to the heterogeneous nucleation and bubble growth process caused by the air in the fuel liquid. The phase change from liquid to vapor requires energy, which is due to the enthalpy of the liquid itself, and the fuel flow in the nozzle seems to involve a temperature drop in addition to the phase change. The speed of sound for liquid is different from the speed of sound for vapor, and the speed of sound for a mixture of vapor and droplet is significantly lower than the speed of sound for both. Therefore, even if the jet velocity is below the speed of sound condition of the liquid, flash boiling spray is underexpansion state in the near-nozzle region, as seen in supersonic jets. In this study, the mass conservation and energy equations of the flash boiling spray were analyzed, and the phase change of the fuel spray at the nozzle exit was quantitatively predicted. In addition, the underexpansion state of the flash boiling spray was analyzed by calculating the speed of sound in the mixture of vapor and droplet from the results of the phase change analysis.

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Multi-physics and Machine Learning Framework for Predicting Air Entrapment During Drop Impact onto Solid Hydrophobic Surfaces

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Key Words: *Phase field model, Machine learning, Drop impact, Air bubble*

One of the fundamental requirements of painting and coating technologies is the controlled and homogeneous deposition onto a solid surface. However, an uncontrolled air bubble entrapment under the deposited liquid layer could deteriorate the quality and durability of a film, and in some cases may cause significant damage. It is challenging to directly monitor the flow details during painting and coating under practical operation conditions. However, simple photographs of a deposited product could shed light on a potential failure, thus allowing to foresee future painting/coating degradation. Predicting such an undesirable air bubble entrapment in advance under real conditions is an imperative step in ensuring high quality painting/coating films. In this contribution, we present a combined multi-physics and deep-learning approach validated by our own experimental measurements to detect air bubble formation during drop impact onto solid parafilm surfaces.

The multi-physics modeling approach is based on the phase-field modeling (PFM) and the Navier-Stokes equations. The PFM is validated against our own experimental measurements in terms of the drop's maximum spreading and rebound height. Then, several cases with varying Weber and Froude numbers are considered to study air entrapment. The PFM results reveal that air may be entrapped under water drops during the initial deposition, as well as during its retraction after maximum spreading. The volume of the entrapped air bubble varies during both processes, significantly affecting drop spreading and rebound height. Furthermore, the simulation results reveal a significant pressure build-up in the entrapped air (up to an order of magnitude higher than that in the surrounding water phase), which has a detrimental effect on drop deposition. Based on our predictions and experimental results a map in the Weber vs. the Froude number plane describing the air entrapment domain is established and discussed.

Using the experimental and multi-physics modeling results, we have further developed a deep-learning approach based upon the VGG16 convolutional neural network (CNN) to predict air bubble entrapment. Hyperparameter optimization is performed to improve the accuracy of the model. It was observed that the CNN, trained based on the experimental images, reveals better predicting capabilities than the one trained based on the simulated images. In addition, for both data sets the prediction is more accurate when training the model using side views rather than the top views. Thus, the present combined deep-learning modeling approach and experimental measurements allow for a fast and precise prediction of air bubble entrapment during drop impact onto solid surfaces.

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Novel Spray Breakup Model with Multi-hole Nozzle in Port Fuel Injection SI Engine

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Key Words: *Port Fuel Injection SI Engine, Fuel Spray Atomization, Breakup Model*

Recently, the electrification of automotive powertrains has been accelerating to achieve a decarbonized society. Meanwhile, it is important to improve the efficiency and low pollution of internal combustion engines, considering that Well to Wheel emissions of CO_2 are lower than those of electric vehicles, and that internal combustion engines are expected to account for 80% of vehicle sales in 2050 [1][2].

Numerical simulations are widely used in the research and development of automotive engines. Spray breakup models in the numerical simulation are important because spray atomization has a significant influence on the subsequent wall impingement behavior and mixture formation. Therefore, the purpose of this study is to investigate the spray atomization process and predict the breakup process in multi-hole nozzle spray for port fuel injection SI engine.

In this study, novel spray breakup model for gasoline spray injected from plate type multi-hole nozzle is developed [3]. This model is considered the liquid sheet breakup based on the phenomenological sheet breakup theory [4]. In this report, this novel breakup model is applied to numerical simulation of fuel spray and predict the spray formation. The validation of the model was carried out by comparing the spatial distribution and the droplet diameter distribution of the fuel spray with experimental results.

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Numerical Analysis of Diesel Hollow Cone Spray Behavior in the Initial Stage of Injection

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Key Words:*Diesel Engine, Computer Fluid Dynamics, Spray Model, Fuel Injection, Atomization*

ABSTRACT

In fuel injection process in diesel engines, the internal nozzle flow has a significant effect on the spray characteristics such as droplet diameter distribution and concentration distribution. Numerical analysis of diesel sprays, the calculation of spray behavior is often carried out without calculating the flow in the nozzle, and the effect of the flow in the nozzle needs to be analyzed as an injection model to predict the spray injection near the nozzle hole. However, almost injection models ignore the unsteady state flow in the nozzle and require the input value of spray angle measured value in the quasi-steady state. Therefore, it is necessary to develop an injection model that can accurately predict the spray injection behavior with internal nozzle flow. The flow in the nozzle has been analyzed experimentally by visualizing the inside of the nozzle and numerically by using commercially fluid simulation code. The behavior of the spray near the nozzle hole has also been investigated by taking magnified images of the spray near the hole. These results indicate that the spray angle increases in the initial stage of the spray due to the effect of swirling flow and string cavitation in the nozzle. In addition, the X-ray spray analysis indicates that a hollow cone spray is formed when the spray angle increases in the initial stage of injection. In this study, a new spray injection model is developed to predict the spray injection behavior near the nozzle hole and the hollow cone spray in the initial stage of injection by considering the flow in the nozzle with minisac type. In the initial stage of injection, the seat throttle mainly affects the injection rate, and after that, the nozzle hole throttle affects the injection rate. Therefore, our one-dimensional model considerd the seat and nozzle hole throttling. By using this model, the pressure in the sac and the angular velocity of the swirling flow in the sac were estimated, and the injection velocity and injection angle were calculated. The initial droplet diameter was calculated by considering the liquid film thickness in the case of hollow cone sprays, and the diameter of the nozzle hole and the contraction flow in the case of solid sprays. The timing of hollow cone sprays was estimated by analyzing the results of sheet scattered light photography of diesel sprays. In addition, the model was applied to KIVA3V, one of the most popular codes for engine in-cylinder analysis, to analyze the diesel spray behavior. The results of the analysis using KIVA3V were compared with the results of diesel spray visualization using sheet scattered light photography, and the accuracy of the model was evaluated.

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On The Shear Atomization Of Thin Liquid Layers

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Key Words: *Atomization, Thin layers, Manifold death, Basilisk*

The atomization of thin liquid layers in closed channels is a process closely related to aerosols generation in several scenarios, such as the respiratory system during coughing and sneezing. This problem has regained relevance lately due to its relation with Covid-19 transmission [1].

In this work, we study the deformation and atomization of a thin liquid layer subject to a rapid air stream in a closed rectangular channel. We run numerical simulations of this setup using the Volume-of-Fluid (VOF) method with octree Adaptive Mesh Refinement (AMR) to capture local small-scale phenomena related to turbulence and breakup. Regarding the latter, we control the impact of grid resolution by applying breakup control by means of a Manifold Death algorithm [2].

We consider different flow regimes, defined by the gas velocity and the liquid viscosity. We compare the droplet-size distribution of these cases with data from experiments with an analogous setup and with measurements taken from real cough experiments. The atomization mechanisms observed in this problem are similar to those of multiphase mixing layer experiments and simulations, resulting in Log-Normal distributions replicated in the experiments. We also report the droplet velocity distribution, analyzing the acceleration of the drops at early atomization stages.

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Vortex driven liquid fragmentation in pressurized liquid injection from multi-hole nozzles

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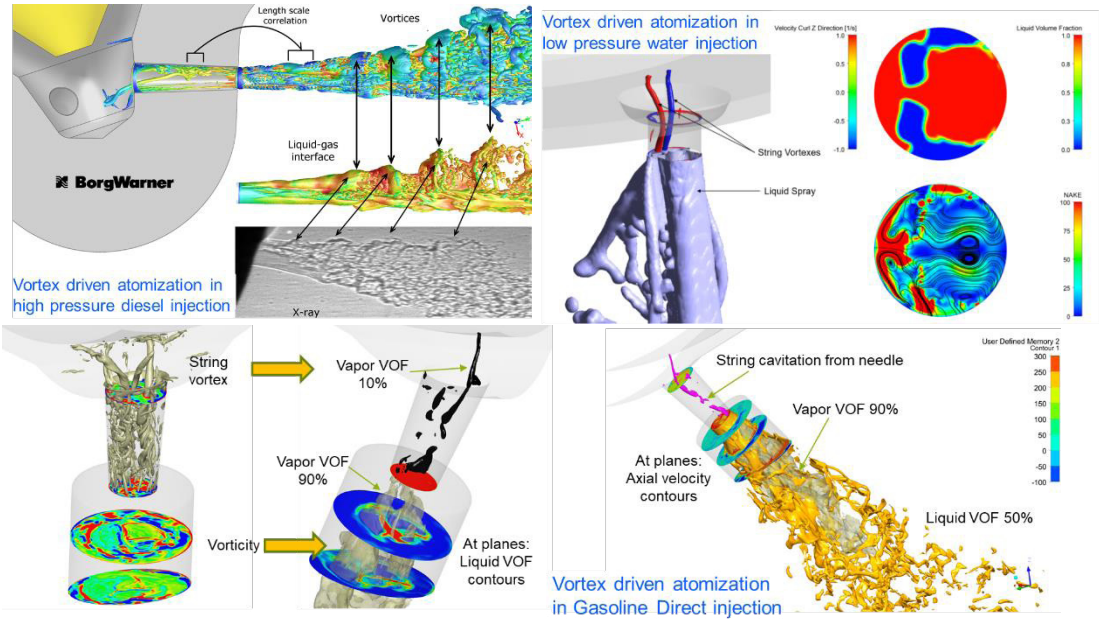
Key Words: *High Pressure Fuel Injection, Low Pressure Water Injection, SCR, Level Set, VOF, LES, Large Scale Vortices, Atomization, Spray Correlation*

Multi-hole pressure atomizers find wide applications in internal combustion engine systems, including high pressure diesel fuel injection (up to 3000 bar), gasoline fuel direct injection (up to 500+ bar), low pressure gasoline port fuel (4-6 bar) or water injection (5-10 bar), and AdBlue injection in the exhaust gas aftertreatment device (5- 10 bar). For all these atomizers, the injection nozzle design has a crucial influence on the engine combustion and exhaust emission performance. Knowledge driven atomizer design requires a understanding of fundamental physics behind the spray formation phenomenon and a continuous search of innovative atomization mechanism. This paper is to present a summary of our research progress on this topic over the past 9 years using Scale-Resolve-Simulation and high resolution micro-visualizations. Although these different applications operate in very different atomization regimes according to established knowledge in literature, they have one thing in common, namely the vortex dynamics in the nozzle flow triggers the liquid jet deformation and ligament formation as an important mechanism driving the near nozzle spray development. Examples will be presented to demonstrate the link between vortex structures, dynamics and the spray structures in the primary breakup regime for the above mentioned different atomizers (e.g. see Figures below). The influence of nozzle design on the vortex flow and spray will also discussed. On the basis of Scale-Resolve Simulations, correlations have been developed between spray penetration, droplet size and nozzle geometry or nozzle flow using URANS simulations and tests.



A Preliminary Numerical Simulation for Flows through Oblique Detonation Engines based on Less Dissipative Schemes and Machine Learning

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Key Words: Oblique Detonation Engines, Detonation Wave, Shock wave, Machine Learning, Detonation Engine.

In this study, an interfacial variable interpolation of ATM (Average of THINC-EM and MUSCL), a hybrid method with the MUSCL interpolation method with the THINC-EM schemes, is proposed to achieve the less numerical dissipative solutions of smooth profile and discontinuities. The main idea of the hybrid approach of ATM is to reconstruct the right and left cell interfacial data by the weighting function of pressure or primitive variable gradients. To determine the optimal weighting parameter settings in the ATM, the Q-learning Q-table method in reinforcement learning is performed on the benchmark test case of the two colliding waves. In addition, the ATM method is extended to solve the stiffened Euler equations to achieve accurate simulation of the detonation waves, shock waves, and the expansion fans for the detonation flow problems. The further performance analysis of the oblique denotation engines will be performed.

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A Time Consistent Method by Preconditioning of the Diffusion Term for Unsteady Gas-Liquid Two-Phase Flows

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Key Words: *Gas-Liquid Two-Phase Flow, Time Consistent Preconditioning, Roe Upwind Scheme, Riemann Problem*

Gas-liquid multiphase flow often happens in hydro machines. In cavitating flow as an example of typical gas-liquid two-phase flow, when its bubble occurs and collapses near body surfaces, it causes the noise, vibration, and damage to the hydro devices. In the sense of reducing these unfavorable effects, in order to clarify and understand the behavior of cavitating flow, several efforts to propose cavitating flow model and numerical method have been made [1,2]. However, due to its strong and complicated unsteady flow phenomenon such as phase changes and the co-existence of compressible and incompressible flow nature, the mathematical model and numerical method is not established yet. Recently, Shin et al. [3] has proposed a preconditioned dual time-stepping method based on a homogenous cavitation model to treat cavitation problems. This method has solved many gas-liquid two phase flow problems associated with wide range of speeds of sound, but relatively it takes time to get the unsteady solution.

In this study, a time consistent preconditioning method for gas-liquid multiphase flows is proposed. A finite-difference 4th-order Runge-Kutta method and a Roe-type flux splitting method with the 3th-order MUSCL TVD scheme are employed. The artificial viscous terms in the flux splitting are modified by using the preconditioning matrix to enhance the numerical stability and accuracy of unsteady computation for compressible and incompressible flow with arbitrary Mach numbers. By using the concept of the homogeneous equilibrium model, gas-liquid two-phase flow is modeled to a pseudo single-phase flow, taking into account the compressibility of the mixed medium. From the above, the present method permits simple treatment of the whole gas-liquid two-phase flow including wave propagation, large density changes, and compressible and incompressible flow characteristics.

As numerical examples, Riemann problems of gas-liquid two-phase shock tube problem were applied to investigate the validity of the present method. From the computation, it showed a good prediction of pressure, density, velocity and void fraction distributions in comparison with Roe's approximate solutions, and quite well simulates unsteady phenomena of the shock wave including the propagation of both compression and expansion waves. The reliability and applicability of the present method to arbitrary Mach number flow problems were confirmed as consequence. Detailed observations of shock and expansion wave behaviors in the gas-liquid media and comparisons of predicted results with exact solutions are provided and discussed.

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An accurate and efficient scheme to capture the sharp interface in high-speed multiphase flow

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Key Words: Two-fluid model, high speed flow, Interface-sharpening

This paper present a single-pressure-field two-fluid model with finite volume discretization to solve the motion of compressible multiphase flow. To resolve both smooth and discontinuous profiles of flow quantities, we proposed a generalized sharpening technique that combines the conventional monotonic upstream scheme for conservation law (MUSCL) and tangent of hyperbola interface capturing (THINC) schemes. A slope-ratio parameter is devised to determine the proportion of values obtained by MUSCL and THINC automatically. Fluxes across cell faces are evaluated by the so called "hybrid AUSMD-type algorithm", where the mass flux and pressure on cell faces are calculated using primitive variable Riemann solver (PVRS). The accuracy and robustness of the proposed scheme are validated by a series of high-speed multiphase flows, where complex wave structures are involved. Unlike the existing scheme (e.g., MUSCL), which usually suffers from numerical diffusion, the proposed scheme significantly sharpens the fluid interfaces and captures more details of wave patterns including shock waves and rarefaction fans. Moreover, for the problem in which surface tension is important, the proposed method shows good capability in increasing the accuracy of curvature estimation. Finally, simulations of a three-dimensional example of the liquid jet crossflow are conducted. The proposed scheme shows more details of the fluid interface, including the interfacial instabilities on the windward side of the liquid jet and droplet formation due to the breakup phenomenon in the downstream of the crossflow, than the existing schemes

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Numerical simulation of two phase flow using general pressure equation

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Key Words: General pressure equation, phase field method, two-phase flow

The general pressure equation-based method[1] is fully explicit, and the method does not require either solving the pressure Poisson equation nor executing sub-iteration for incompressible flow simulation. In this work, general pressure equation based method is used to conduct numerical simulations of two phase flows using phase field method[2] coupled with level set method[3]. Several test problems are used to demonstrate the capability of the current approach. The simulations are conducted on GPU cluster using MPI and CUDA[1, 4].

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Folding Instabilities in Viscoplastic Sheets

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Key Words: *viscoplastic fluids, yield stress, folding instabilities, rheology*

In this work, we investigate viscoplastic effects on the development of folding instabilities in non-Newtonian viscous sheets of fluid which viscosity is given by a Herschel-Bulkley constitutive equation. Such instabilities are trigged by compression stresses acting on viscous sheets that comes out of a channel at a very small initial velocity, fall, and then hit a solid surface or a fluid substrate. Our study is conducted through a mixed approach combining direct numerical simulations, energy budget analyses, scaling laws, and experiments.

The numerical results are based on an adaptive variational multi-scale method for multiphase flows, while Carpobol gel, ketchup and mayonnaise sheets are used for the lab experiments. Three folding regimes are observed: (1) the viscous regime; (2) the plasto-gravitational; and (3) the visco-gravitational one. Interestingly, only the second and the third mentioned regime are affected by non-Newtonian manifestations within the material. In short, when gravity is balanced by viscoplastic forces along the non-Newtonian viscous sheet, both the folding amplitude and the folding frequency are given by a Herschel-Bulkley function of the sheet slenderness, the Galileo number (the ratio of the gravitational stress to the viscous one), the Bingham number (the ratio of the yield-stress and the gravitational one) and the flow behaviour index of the constitutive law. Highly plastic materials develop large amplitude (and low frequency) instabilities, which, in contrast, tend to be suppressed by shear thinning effects, and eventually cease. Lastly, non-Newtonian effects on folding onset/cessation are also carefully explored. As a result, non-Newtonian folding onset and cessation criteria are presented.

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A Consistent, Explicit and Accessible Boltzmann Collision Operator for Polyatomic Gases

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Key Words: kinetic transport, mathematical modeling, fluid dynamics, partial differential equations

While the kinetic theory of monatomic gases is complete, modelling the kinetic transport of polyatomic gases remains challenging. This is mostly due to the much more complicated particle interaction which is modeled as simplified relaxation to equilibrium in most kinetic equations nowadays, e.g., in [3].

Based on a continuous internal energy state variable, we propose an explicit, fully non-linear Boltzmann collision operator for the evolution of distribution function describing a polyatomic gas with constant heat capacity [1]. The particle interaction is a polyatomic generalization of the variable hard sphere model, used in a recent rigorous mathematical analysis [2], and includes frozen collisions. The model is consistent with the monatomic case and allows easy evaluations for moment equations and the Chapman-Enskog expansion. Using a specifically tailored computer algebra code, which is publicly shared, we can explicitly compute nonlinear production terms for macroscopic systems of moments. The range of Prandtl number values recovers the Eucken formula for a specific choice of parameters. The new collision model allows on the one side to study differential cross sections and how the dependencies on relative velocity and internal energies of the polyatomic particles influences macroscopic fluid properties.

On the other side moment equations as in [3] can be derived with explicit production terms obtained from the new collision operator. We will discuss preliminary results from the polyatomic hierarchical moment cascade for heat conduction in the spirit of [4].

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Convergence and Error Estimates for the Conservative Spectral Method for Fokker-Planck-Landau Equations

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Key Words: Fokker-Planck-Landau, Type Equations; Boltzmann Equation; Numerical Schemes; Conservative Spectral Methods; Error Estimates; Numerical Analysis

Error estimates are rigorously derived for a semi-discrete version of a conservative spectral method [1,2] for approximating the space-homogeneous Fokker-Planck-Landau (FPL) equation modeling a probability density function associated to hard potentials [1]. The analysis, inspired by the work in [4], consists in showing properties of the semi-discrete scheme is consistent, conservative, it has a unique semi discrete solution with bounded moments depending on the initial data and the computational domain, and local time stability converging to the approximating stationary state given by the global Maxwellian probability density distribution. In addition, the derivatives of such solution, up to any order, also remain bounded in Sobolev spaces for three dimensional local velocities and globally in time. The estimates depend on the initial model data and the computational domain, as expected to be for kinetic collisional models.

These estimates, combined with control of the spectral projection, are enough to obtain error estimates to the analytical solution and convergence to equilibrium states. It is noted that this is the first time that an error estimate has been produced for any numerical method which approximates FPL equations associated to any range of potentials. Simulations of the space dependent and homogeneous showing the accurate decay to equilibrium for hard potentials and Coulomb interactions will be presented.

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Extending the BGK model: velocity dependent collision frequency and quantum description

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Key Words: BGK approximation, velocity-dependent collision frequency, entropy minimization

The fundamental model I am considering is the so called Bathnagar-Gross-Krook (BGK) equation:

$$\partial_t f + v\nabla_x \cdot f = \nu(M(f) - f)$$

where f is the distribution function of the gas, $M(f)$ the equilibrium distribution (in the classical case a Maxwell distribution) and ν describes the collision frequency. The BGK equation is an approximation of the Boltzmann equation which has the same main properties as Boltzmann (conservation of properties, H-Theorem and the same shape of the equilibrium) and is much more efficient in numerical simulations. Therefore, in many applications, this approximation is used. However, the standard BGK equation is too simple in real applications. Therefore a recent open question is if it is possible to equip this approximation with more physics to describe more complex phenomena but still try to keep the numerical efficiency.

In this talk, I will focus on including a velocity dependency into the collision frequency and quantum effects. In both cases the Maxwell distribution has to be exchanged by a different function which leads to difficulties in the proof of the conservation properties and the H-Theorem.

Finally, I will give an outlook for extending this strategy to cover a large class of BGK models including for example the quantum BGK model with velocity dependent collision frequency, the relativistic BGK model with velocity dependent collision frequency, BGK models for gas mixtures and BGK models for polyatomic molecules.

This is joint work with S. Yun, G. Bae, (Sungkyunkwan University), J. Haack (Los Alamos National Laboratory), C. Hauck (Oak Ridge National Laboratory) and C. Klingenberg, S. Warnecke

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Numerical Analysis of a Slow Rarefied Gas Flow past a Circular Disk

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Key Words: Rarefied Gas, Non-Continuum Flows, Method of Characteristics

The slow uniform flow past an object is one of the fundamental problems in rarefied gas dynamics and plays a vital role in MEMS and aerosol transport. In the case in which the obstacle is a spherical body, a hybrid scheme for the Boltzmann equation, combining the finite difference method and the method of characteristics, was successfully applied, and detailed flow structures were clarified (e.g., [1]). On the other hand, the analysis of the flow past a three-dimensional object with a sharp edge, such as a disk, is much less developed. In this case, the high dimensionality and the complex structure of the velocity distribution function (VDF) make the hybrid method impossible to apply in practice.

In this study, we consider a uniform flow of a rarefied gas past a circular disk. More precisely, we investigate the steady behavior of the gas around the disk based on the Bhatnagar–Gross–Krook (BGK) model of the Boltzmann equation and the diffuse reflection boundary condition under the linearization. Our strategy is to solve an integral equation for an unknown function (VDF) derived by applying the method of characteristics. At first glance, this approach seems inefficient as compared to the finite difference method. However, it provides more flexibility in generating the mesh for numerical integration, which is important for capturing the discontinuity in the VDF, as demonstrated in moving boundary problems [2] and time-dependent problems [3].

The numerical solutions are obtained for various values of the Knudsen number, i.e., the ratio between the mean free path of the gas molecules at the reference equilibrium state and the radius of the disk. The details of the macroscopic profiles and the precise value of the drag will be presented in the talk. The present study shows that the numerical analysis based on the method of characteristics is now feasible for three-dimensional external flow problems with sharp edges with reasonable computational resources.

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On scientific machine learning of kinetic theory and fluid dynamics

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In this talk, I will introduce the momentum built by machine learning methods in computational sciences. Specific attention will be paid on the usage of deep neural networks as building blocks in a numerical method to solve the Boltzmann-type kinetic equations. This is a particularly interesting topic since the high-dimensional integro-differential equation possesses an intricate structure that a numerical method needs to preserve. As universal function approximator, artificial neural networks might be beneficial but cannot be used out-of-the-box. The ongoing project is dedicated to touches upon the applications point of view of deep learning with a focus on interpretability and robustness, and on the mathematical methodologies point of view to solve partial differential equations. The following figures show the preliminary work on this research topic.

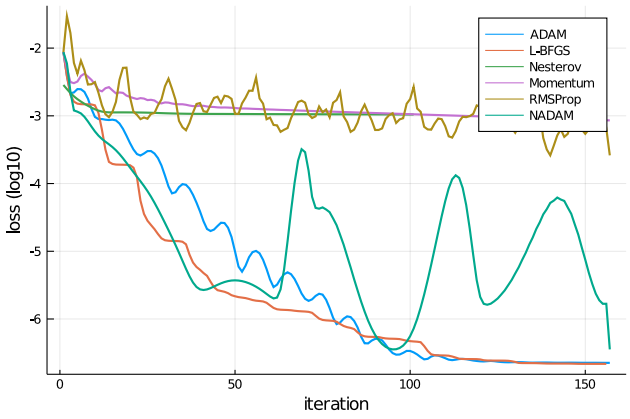

Figure 1: Iterations of loss with different optimizers.

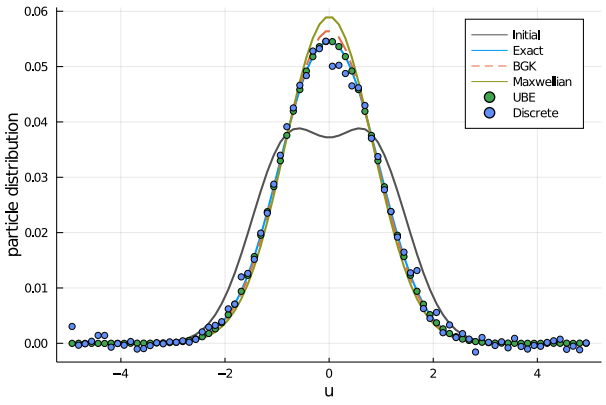

Figure 2: relaxation of non-equilibrium particle distribution.

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On the kinetic model for a polyatomic gas: the Cauchy problem and moment equations

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This talk focuses on the Boltzmann equation that models a polyatomic gas by introducing one additional continuous variable, referred to as microscopic internal energy [1, 2]. We will discuss the existence and uniqueness theory in the space homogeneous setting for the full non-linear case, under an extended Grad assumption on transition probability rates, that comprises hard potentials for both the relative speed and internal energy with the rate in the interval (0, 2], which is multiplied by an integrable angular part and integrable partition functions [3].

The Cauchy problem is resolved by means of an abstract ODE theory in Banach spaces, for an initial data with finite and strictly positive gas mass and energy, finite momentum, and additionally finite $k*$ polynomial moment, with $k*$ depending on the rate of the transition probability and the structure of a polyatomic molecule or its internal degrees of freedom. Moreover, we will prove that polynomial and exponential moments associated to the solution are both generated and propagated.

Based on this kinetic model, we will build moment equations. The transition probability rate proposed in [3] is shown to provide an accurate macroscopic theory and to recover physical properties such as the Eucken formula for the Prandtl number and experimentally observed viscosity dependence upon temperature [4–6].

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Quasilinear Diffusion of magnetized fast electrons in a mean field of quasi-particle waves packets

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Key Words: Quasilinear Theory, Mean Field Theory, Finite Element Method

Quasi-linear diffusion of magnetized fast electrons in momentum space results from stimulated emission and absorption of waves packets via wave-particle resonances. Such model consists in solving the dynamics of a system of relativistic kinetic diffusion processes described by the balance equations for electron probability density functions (electron pdf) coupled to the time dynamics waves (quasi-particles) in a quantum process of their resonant interaction. Such description results in a Mean Field model where diffusion coefficients are determined by the local spectral energy density of excited waves whose perturbations depend on flux averages of the electron pdf, introduced in [1], [2], [3].

We will discuss the model and a mean field iteration scheme that simulates the dynamics of the space average model, where the energy spectrum of the excited wave time dynamics is calculated with a coefficient that depends on the electron pdf flux at a previous time step; while the time dynamics of the quasilinear model for the electron pdf is calculated by the spectral average of the quasi-particle wave under a classical resonant condition where the plasma wave frequencies couples the spectral energy to the momentum variable of the electron pdf. Recent numerical simulations will be presented showing a strong hot tail anisotropy formation and stabilization for the iteration in the relativistic 3 dimensional cylindrical coordinates model.

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A Discrete Exterior Calculus Based Framework for CFD

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Key Words: *Discrete exterior calculus, vortex dynamics, multiphase flows, Solar Convection.*

Exterior calculus is a generalization of vector calculus to manifolds of arbitrary dimension. Discrete exterior calculus (DEC) [1] is the discrete version of exterior calculus. In DEC, physical fields are discretely expressed as *k*-forms representing the integration of the physical quantity on k-dimensional primal/dual mesh objects. DEC ensures that vector calculus properties are discretely satisfied. In addition to preserving the mathematical properties it allows for conservation of secondary quantities, such as kinetic energy and vorticity for an inviscid flow [2]. DEC is coordinate independent, and convenient for investigating flows over curved surfaces.

We present a framework for computing flows on surfaces based on a DEC discretization of Navier-Stokes (N-S) equations on simplicial meshes. The framework incorporates rotational and primitive formulations of the NS equations and allows for different time integration methods including those which feature energy conservation [3]. Other features of the framework consist of the inclusion of the Coriolis force term to investigate flows on rotating surfaces, and phase-field based interface tracking methods for multiphase flows. Moreover, we have enhanced our DEC framework to build hybrid DEC-FD and DEC-FFT discretizations which are useful for the investigation of convection in spherical shells and aerodynamic flows, respectively. The method is second order accurate on structured triangular meshes, and first order on otherwise unstructured meshes. It demonstrates the conservation of inviscid invariants such as kinetic energy and enstrophy over an extended period of time [4].

We present simulation results for a variety of physical configurations including the flow past a circular cylinder and airfoils, multiphase flows, vortex dominated flows on surfaces with and without rotation, and convection in spherical shells.

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Large Eddy Simulation and Hybrid RANS/LES of Heat transfer for Staggered Pin-Fin Matrix

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Key Words: *Large eddy simulation(LES), Stress blended eddy simulation(SBES), Improved delayed detached eddy simulation(IDDES) CFD, Heat transfer, Pin-Fin matrix,*

The pin-fin matrix is adopted representatively in heat exchanger, turbine blade and nuclear reactor to improve the performance of heat transfer. The structure of the pin-fin matrix seems to be simple, but heat and flow structure are complicate. In this reason, many researchers have investigated the heat transfer phenomenon. First of all, Ames et al.[1] conducted an heat transfer experiment on staggered pin-fin matrix with hot wire and infrared camera. Reynolds number 3,000, 10,000 and 30,000 were investigated. Benhamadouche et al.[2] conducted numerical simulation for staggered pin-fin matrix with 4 turbulence model (k - ω SST, ϕ - model, EB-RSM, LES).

In present work, two hybrid RANS/LES models and one LES model are adopted to study heat transfer and fluid flow on staggered pin-fin matrix at Reynolds number, 10,000. Two hybrid RANS/LES modes are an improved detached eddy simulation (IDDES) and a stress-blended eddy simulation (SBES). The LES model is based on dynamic Lily model. 3D vortical flow structures and turbulnece properties were compared depending on the adopted models. Also heat transfer properties including averaged Nusselt number at each surface was presented with comparison of experimental data[1].

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Multi-Region and Multi-Component Thermal Fluid Analysis of Hydrothermal Oxidative Decomposition Reactor

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Key Words: *Polychlorinated Biphenyl, Hydrothermal Destruction Reactor, Multi-Region Analysis, OpenFOAM*

Hydrothermal oxidative decomposition is one of methods for detoxification of polychlorinated biphenyls (PCBs, $C_{12}H_{(10-n)}Cl_n$), which are decomposed into water (H_2O), carbon dioxide (CO_2) and sodium chloride (NaCl) by dechlorination with sodium carbonate (Na_2CO_3) and oxidative decomposition with liquid oxygen (O_2) under high temperature 370 °C and high pressure 26.5 MPa [1]. In these reactor vessels, wall thinning due to corrosion was observed on bottom inner wall. At present, the reactors have been safely maintained and operated by adding a bottom partition to prevent chemical sinking and supplying hot water to the reactor vessel bottom to control the temperature. Thermal fluid analysis of the hydrothermal oxidative destruction reactors is necessary to clarify the corrosion mechanism.

A finite volume analysis solver chtMultiRegionTwoPhaseEulerFoam of OpenFOAM [2] is used to perform a multi-regionally coupled analysis of the internal fluid flow and heat conduction in the reactor vessel considering the conjugate heat transfer on the solid-liquid interface. The internal fluid is two-component fluid, PCB and water, with different densities without chemical reaction. Advection equation for the volume fraction of two fluids, compressible Navier-Stokes equation with gravity term, and energy equation are staggeringly solved for unsteady thermal fluid analysis. The Reynolds-averaged Navier-Stokes equations based on the standard k-ε model are used for turbulent flow analysis. Temperature dependent thermo-physical properties of PCB and water such as specific heat, thermal conductivity and viscosity, and equation of state of density, are employed as polynomial equation of temperature.

As a result of the analysis, the density difference flow of the two fluids was confirmed. To evaluate the integrity of the hydrothermal oxidative destruction reactor vessel, corrosion risk was evaluated based on the results obtained from the analysis such as temperature, volume fraction of PCB and wall shear stress on the solid-liquid interface.

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Numerical Study of the Heat Transfer Process in a Wind Tank

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Key Words: Heat Transfer, CFD, Thermal Comfort, Wind Tower, Wind Tank

In regions with a warm climate, the demands for thermal comfort also imply high consumption of electrical energy. The actual enviromental situation and the climate change impose a challenge in using renewable sources of energy in order to achieve thermal comfort for living spaces located in regions of hot/warm climate such as the tropics.

A solution that uses renewable energy is a wind tank; which is a structure located in the upper part of a living space (e.g: a house) with a compartment for water storage and with lower lateral openings that allow the air flow through water distribution line pipes acting like heat exchangers to cool the living space [4]. With the use of elevated tanks acting like wind towers [2], thermal comfort would be improved at times of the day with higher temperatures when the wind is favorable. To achieve the above, it is necessary to know the relevance of airflow [3] and heat transfer [1] through the installed water distribution lines that act as heat exchangers. A three-dimensional CFD simulation was performed to study the distribution of temperature, velocity and pressure due to the wind tank in a test room; three different wind tanks were analyzed varying their height above the roof. The natural tendency of the air to flow through the wind tank and its exit through the room windows is confirmed; the internal velocities reached acceptable average values, and heat transfer from air to water distribution lines allows cooling the room to acceptable levels for thermal comfort. The presence of heat exchangers causes drops in circulating air pressure but leaves enough fresh air inlet. A sensibility study was realized to find the influence of water temperature in living space thermal comfort.

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Optimal Cooling Design of Gamma-ray Converter with Venturi Structure Based on Multi-physics Analysis

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Key Words: *Multi-physics analysis, Particle accelerator, Venturi structure*

In recent years, a new method to produce Mo-99 with a particle accelerator, which emits less amount of nuclear waste than nuclear reactor, gets a lot of attention [1]. In this method, accelerated electron beam is generated, converted into gamma-ray, irradiated onto the specimen and then Mo99 is obtained. Here, it is important to cool the gamma-ray converter made of copper alloy plates, which are exposed to large heat loads. For more efficient cooling, forced convection of water is adopted, where the converter itself is used as the flow channel.

To enhance the cooling effect, higher Reynolds number and large surface area are effective. However, the converter channel has design constraints on flow rate and the volume irradiated by the beam. For this reason, we focused on the flow control using venturi structure. There are few studies that applies venturi structure to cooling design. Hatami et al. [2] numerically investigated the effect of venturi tube on the cooling performance of nanofluid.

Venturi structure is composed of two sections: nozzle section and diffuser section. In the nozzle section, the width of the channel gradually decreases, and the flow velocity increases. In the diffuser section, the width is restored to the original value, and turbulence is more likely to occur. Applying this structure to the upstream, local turbulence with high flow velocity can hit the heated part of converter.

Venturi structure has three design parameters: nozzle length l_n, nozzle equivalent diameter d, diffuser length l_d. By experimental design, various combinations of these design variables are prepared. Then, each design proposal is analysed using multi-physics analysis of LS-DYNA R12. The conjugate heat transfer between structure and fluid is calculated, and the maximum temperature of each design is extracted as the objective variable. In the analysis, constant volumetric heat generation is imposed on the heated part of converter, and the flow rate is set constant.

As a result, a design proposal with stepped-shape diffuser ($l_d = 0$) showed the highest cooling performance. The optimal design effectively accelerates the flow and guide the high-velocity turbulent flow to hit the surface of heated part. This leads to 6.2 % decrease of the maximum temperature when the converter is irradiated by 10 kW electron beam, compared to the base design with flat channel.

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Transient cooling of reactor vessel wall during LOCA

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Key Words: *CFD, FVM, PTS, LOCA*

The article describes a multistage modelling methodology proposed by the author for the modelling of emergency core cooling processes. The methodology is based on the best practice guidelines presented by the IAEA, it is applied to a specific scenario of emergency core cooling during a loss of coolant accident[1] with an effective break diameter of 20mm.

A 3D thermohydraulic analysis was performed as the first step in the solution process, where the transient changes in the pressure, velocity and temperature fields within the reactor pressure vessel were studied [2]. The transient CFD analysis simulated the fluid structure interaction between the coolant and the reactor pressure vessel wall. This interaction focused on the thermal field and the unsteady cooling processes. The primary knowledge learned when processing the results of the first step, was the presence of an oscillating cold coolant stripe in close proximity to the pressure vessel wall.

The next step in the methodology consisted of a three-dimensional thermo-mechanical analysis of the reactor pressure vessel [3]. In this step, pressure thermal shock induced critical zones of mechanical loading were identified and the influence of the oscillatory character of the cold stripe on the pressure vessel was studied.

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Accelerating Structural and Fracture Mechanics Simulations with Localised Phenomena through Matrix Compression and Sub-Structuring

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Key Words: model order reduction, localised damage, Hierarchically Off-Diagonal Low Rank (HODLR) approximation, dynamic substructuring

Several problems in structural and fracture mechanics involve stationary or evolving localised features, such as cracks and damage. A repetitive solution of the forward equations of these problems is often required, to track for instance the evolution of damage for different system configurations, or as part of an inverse problem solution. In such settings, that are often encountered in the realms of Structural Health Monitoring (SHM) and reliability assessment, significant benefits are attained from the use of model order reduction, to decrease the associated computational cost. However, conventional projection-based techniques, which are often preferred for reduction, would not be effective for such problems due to the infeasible size of the resulting parameter spaces, which should account for all possible feature locations and configurations [1], as well as additional parameters, such as environmental and operational conditions.

In the present work, an alternative approach is proposed, where low-dimensional spaces, created for the original system, in the absence of localised features, are enriched with appropriately selected columns of the flexibility matrix of the system. While it can be shown that this approach exactly recovers the solution of the full order problem in the static case, its application for general localised features requires the computation of the full flexibility matrix of the system, which can quickly become intractable in terms of memory. This issue is mitigated by using a Hierarchically Off-Diagonal Low Rank (HODLR) representation for the involved system matrices [2], while the computational cost, which depends on the size of the flexibility matrix, is further reduced by means of dynamic substructuring [3]. This allows to effectively scale the computational time by only extracting the flexibility matrices of the sub-structures, whose size is much more reduced than the one of the full-order system. The efficiency of the resulting scheme is demonstrated through a series of numerical applications, involving large-scale structural dynamics models with localised damage.

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Accurate and Robust Splitting Methods for the Generalized Langevin Equation with a Positive Prony Series Memory Kernel

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Key Words: *Stochastic Differential Equations, Splitting Methods, Generalized Langevin Equation, Memory Kernel, Error Analysis, Harmonic Oscillator*

We study numerical methods for the generalized Langevin equation (GLE) with a positive Prony series memory kernel, in which case the GLE can be written in an extended variable Markovian formalism. We propose a new splitting method that is easy to implement and is able to substantially improve the accuracy and robustness of GLE simulations in a wide range of the parameters. An error analysis is performed in the case of a one-dimensional harmonic oscillator, revealing that all but one averages are exact for the newly proposed method. Various numerical experiments in both equilibrium and nonequilibrium simulations are also conducted to demonstrate the superiority of the newly proposed method over popular alternative schemes in interacting multi-particle systems.

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Adaptive Multigrid Strategy for Large-scale Molecular Mechanics Optimization

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Key Words: *adaptive multigrid, molecular mechanics, large scale optimization, a posteriori*

We present several efficient adaptive multigrid strategies for large-scale molecular mechanics optimization. The oneway multigrid method is used with inexact approximations at every coarse level and the adaptive quasi-atomistic approximation and the adaptive blended ghost force correction (BGFC) method are considered as the coarse-grid problems. Mesh refinements based on the gradient-based a posteriori error estimator can obtain better approximations on the coarse-grained levels. Sublinear complexity is observed numerically when the BGFC method is used for crystals with defects, like vacancies, micro-crack and dislocation. For systems with more than ten millions atoms, this strategy has a fivefold acceleration in terms of CPU time on average.

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Adaptive Parareal Algorithms for Molecular Dynamics Simulations

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Key Words: Molecular dynamics simulation, Stochastic differential equations, Parallel-in-time algorithms, Long time integration

In this talk, we introduce parareal algorithms in the context of molecular dynamics, where we couple a fine propagator based on the reference potential energy landscape with a coarse propagator based on a surrogate potential. Although the parareal algorithm, in its original formulation, always converges, it suffers from various limitations in the context of molecular dynamics. In particular, it is observed that the algorithm does not provide any computational gain in terms of wall-clock time (compared to a standard sequential integration) in the limit of increasingly long time-horizons. This numerical observation is backed up with theoretical discussions. We then introduce a modified version of the parareal algorithm wherein the algorithm adaptively divides the entire time-horizon into smaller time slabs [1]. We numerically show that the adaptive algorithm overcomes the various limitations of the standard parareal algorithm, thereby allowing for significantly improved gains. Several numerical examples will be discussed, including the simulation of defects in tungsten using LAMMPS.

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ATOMISTIC ORIGINS OF CONTINUUM DISLOCATION DYNAMICS

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Key Words: Dislocations, particle system, SDE, mean-field limit, discrete-to-continuum limit

We focus on the connections between four stochastic and deterministic models for the motion of straight screw dislocations. Starting from a description of screw dislocation motion as interacting random walks on a lattice, we prove explicit estimates of the distance between solutions of this model, an SDE system for the dislocation positions, and two deterministic mean-field models describing the dislocation density. The proof of these estimates uses a collection of various techniques in analysis and probability theory, including a novel approach to establish propagation-of-chaos on a spatially discrete model. The estimates are non-asymptotic and explicit in terms of four parameters: the lattice spacing, the number of dislocations, the dislocation core size, and the temperature. This work is a first step in exploring this parameter space with the ultimate aim to connect and quantify the relationships between the many different dislocation models present in the literature.

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Coarse-graining of Markov chains

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Key Words: Coarse-graining, continuous-time Markov chains, fast-slow systems

Various physical phenomenon, such as Markov state models in molecular dynamics, stochastic chemical kinetics for a chemical-reaction system and agent-based models in social dynamics are modelled by jump processes. Coarse-graining of such models has received considerable attention from practitioners in recent years – for instance to perform a data-driven identification of the transition-rate matrix for a reduced set of stable configurations in a molecular system or to deduce subnetwork dynamics from large-scale biochemical systems. Typically in these settings, coarse-graining is characterised by a projection onto a smaller subset of states, which captures the essential slow-behaviour of the model. Inspired by the conditional-expectation closures introduced in coarse-graining of diffusion processes, in this work we propose an *effective dynamics* for continuous-time Markov chains. The central aim of this work is to understand if and when this effective dynamics is indeed a good lower-dimensional approximation of the full stochastic jump process. Using entropy techniques we provide sufficient conditions under which this effective dynamics stays close to the original system and provide quantitative bounds on the approximation error. Furthermore, we connect the effective dynamics to the averaging literature which deals with multi-scale problems in jump processes.

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Data-based model reduction and Mori-Zwanzig formalism for random dynamical systems

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Key Words: Model reduction; Koopman operators; Mori-Zwanzig formalism; nonlinear time series analysis; system identification

The Mori-Zwanzig (MZ) projection operator formalism provides a general framework for constructing reduced models for chaotic and stochastic dynamical systems, particularly in situations without sharp scale separation and hence significant memory effects. In this talk, I will report on an approach to data-based model reduction for stochastic and random dynamical systems using the NARMAX (Nonlinear Auto-Regressive Moving Average with eXogenous inputs) representation of stochastic processes, widely used in time series analysis and data-driven modeling. I will explain how the NARMAX approach may be formally derived from the original dynamical model using a discrete-time version of the MZ formalism. These ideas are illustrated on a stochastically-forced PDE. Time permitting, I will also discuss our recent efforts to improve the efficiency and scalability of our data-based modeling procedure.

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Discretizing Atomistic Dynamics with Markov Renewal Processes

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Key Words: *Long-time dynamics, jump processes, coarse-graining*

Atomistic simulations with methods such as molecular dynamics are extremely powerful tools to understand nanoscale dynamical behavior. The resulting trajectories, by the virtue of being embedded in a high-dimensional configuration space, can however be difficult to analyze and interpret. This makes low-dimensional representations, especially in terms of discrete jump processes, extremely valuable. This simplicity can however come at the cost of accuracy, as tractable representations often entail simplifying assumptions that are not guaranteed to be realized in practice, no matter how the discrete states are defined. We describe a discretization scheme for continuous trajectories that enables an arbitrarily accurate representation in terms of a Markov Renewal Process over a discrete state space. The accuracy of the model converges exponentially fast as a function of a continuous parameter that has the interpretation of a local correlation time of the dynamics, for any state definition.

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Grassmann Extrapolation of Density Matrices for Born-Oppenheimer Molecular Dynamics

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Key Words: Grassmann extrapolation, ab-initio molecular dynamics, QM/MM

Simulating ab-initio molecular dynamics is in general numerically very expensive due to the large non-linear eigenvalue problem that needs to be solved at each time step of the dynamics. This problem is usually solved by means of a self-consistent field algorithm, in which the accuracy of the initial guess strongly influences the number of iterations to perform, and therefore the overall cost of the method.

In this talk, I will present a method for computing accurate initial guesses for the density matrix initiating a self-consistent field algorithm in a Born-Oppenheimer molecular dynamics, based on density matrices at previous time steps. To perform the extrapolation, we introduce a locally bijective map between the manifold where the density matrix is defined and its tangent space so that it is possible to perform linear extrapolation in a vector space, keeping the correct physical properties for the initial guess. I will then illustrate the method with numerical simulations on a few molecules, demonstrating the low computational cost and accuracy of the proposed method.

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Large Deviations for Model Coarse-graining: Metastable Atmospheric Jets

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Key Words: Slow-fast systems, large deviation theory, rare events, metastability, atmospheric flows

In stochastic systems with time-scale separation the average behavior of the effective slow variables can be computed rigorously by stochastic averaging and homogenization. The result is a law-of-large-number type result describing the limiting evolution equation in the limit of infinite time-scale separation. Similarly, typical fluctuations around this most likely behavior can be quantified through a central limit theorem, so that effective stochastic dynamics for the slow degrees of freedom can be derived.

Here we show that these considerations do not contain extremely long-time behavior, such as metastability on the slow time scale, which necessitates macroscopic fluctuations of the slow variable away from its typical behavior [1]. Classical results [2] prove that the corresponding large deviation principle (LDP) involves an Hamilton-Jacobi equation whose Hamiltonian is related to the leading eigenvalue of the generator of the fast process, and is typically non-quadratic in the momenta—in other words, the LDP for the slow variables in fast-slow systems is different in general from that of any stochastic differential equation (SDE) one would write for the slow variables alone. In short, large fluctuations of the slow variables cannot be described by classical Freidlin-Wentzell theory of SDEs.

This situation is not only of mere theoretical interests, but occurs in real-world systems such as atmospheric flow: Here, the slow evolution of atmospheric jets is driven by fast fluctuations of the turbulent flow, and can be approximated by quasi-linear theory. In certain parameter regimes, different arrangements of planetary jets are simultaneously locally stable, and rare fluctuations can drive the system between these states on very long time-scales.

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OPTIMAL RENORMALIZATION OF MULTISCALE SYSTEMS

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Key Words: Model reduction, renormalization, multiscale

While model order reduction is a promising approach in dealing with multi-scale time-dependent systems that are too large or too expensive to simulate for long times, the resulting reduced order models can suffer from instabilities. We have recently developed a time-dependent renormalization approach to stabilize such reduced models. In the current work, we extend this framework by introducing a parameter that controls the time-decay of the memory of such models and optimally select this parameter based on limited fully resolved simulations. First, we demonstrate our framework on the inviscid Burgers equation whose solution develops a finite-time singularity. Our renormalized reduced order models are stable and accurate for long times while using for their calibration only data from a full order simulation before the occurrence of the singularity. Furthermore, we apply this framework to the 3D Euler equations of incompressible fluid flow, where the problem of finite-time singularity formation is still open and where brute force simulation is only feasible for short times. Our approach allows us to obtain a perturbatively renormalizable model which is stable for long times and includes all the complex effects present in the 3D Euler dynamics. We find that, in each application, the renormalization coefficients display algebraic decay with increasing resolution, and that the parameter which controls the time-decay of the memory is problem-dependent [1].

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Solving High-Dimensional Eigenvalue PDEs using Artificial Neural Networks and its Application in Understanding Metastable Diffusion Processes on Large Timescales

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Key Words: Eigenvalue PDE, Metastable Diffusion Process, Artificial Neural Network

Abstract: In this talk, we consider the eigenvalue PDE problem of the infinitesimal generators of metastable diffusion processes. We present a numerical algorithm based on training artificial neural networks for solving the leading eigenvalues and eigenfunctions of such high-dimensional eigenvalue problem. The algorithm is useful in understanding the dynamical behaviors of metastable processes on large timescales. We demonstrate the capability of our algorithm on a high-dimensional model problem, and on the simple molecular system alanine dipeptide. This talk is based on joint work with Tiejun Li and Christof Schütte.

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Tensor-valued Atomic cluster expansion for inference of dynamical systems

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Key Words: Atomic cluster expansion, Dynamical systems, Tensor-valued functions, equivariant basis construction

Complex physical systems are commonly parametrized by tensor-valued coefficients that are functions of the current state of the system. For example, rigorous derivation of the dynamics via the Mori-Zwanzig projection formalism of coarse-grained atomistic systems typically results in a (generalized) Langevin equation with configuration-dependent friction and diffusion coefficients. Learning the dynamics of such systems from data and simulating the inferred model requires efficient parametric representations of such tensor-valued functions. More specifically, such representations should allow for computationally efficient evaluation and data-efficient estimation of their parametrization from data.

The framework of the recently proposed Atomic Cluster Expansion (ACE) [1, 2] has been successfully used for inference of potential energy surfaces and force fields of atomistic systems from data. In this talk, I will present some recent work that was performed in collaboration with C. Ortner which extends the framework of the Atomic Cluster Expansion to equivariant tensor-valued functions. I will discuss the derivation of the resulting basis expansions for matrix-valued and vector-valued functions. Moreover, I will present the results obtained by applying our approach to atomistic trajectory data.

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A Variational Approach based on Perturbed Eigenvalue Analysis for Improving Spectral Properties of Isogeometric Multipatch Discretizations

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Key Words: Isogeometric analysis, outlier frequencies, outlier modes, perturbed eigenvalue analysis, multipatch discretizations, explicit dynamics, critical time step

A key advantage of isogeometric discretizations is their accurate and well-behaved eigenfrequencies and eigenmodes. For degree two and higher, however, the so-called optical branches formed by spurious outlier frequencies and modes may appear due to boundaries or reduced continuity at patch interfaces [1, 2]. The outlier frequencies are significantly overestimated, which unnecessarily reduce the stable critical time-step size in explicit dynamics calculations. Moreover, the outlier modes behave in a spurious manner and may have a negative impact on the solution accuracy and robustness, particularly in hyperbolic problems [3]. In this talk, we present (a) a variational approach based on perturbed eigenvalue analysis to improve the spectral properties of isogeometric multipatch discretizations; and (b) a scheme for estimating optimal scaling parameters of the added perturbation term such that the outlier frequencies are effectively reduced and the accuracy in the remainder of the spectrum and modes is not negatively affected; and (c) how to cast this scheme into a pragmatic iterative procedure that can be readily implemented in any isogeometric analysis framework. We verify numerically via spectral analysis of second- and fourth-order problems that the proposed approach improves spectral properties of isogeometric multipatch discretizations in the one- and multidimensional setting. For exemplary membrane and plate-like structures, we confirm that our approach maintains spatial accuracy and enables a larger critical time-step size. We also demonstrate that it does not depend on the polynomial degree of spline basis functions.

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Auxiliary Splines Space Preconditioning for B-Splines Finite Elements: The case of $\boldsymbol{H}(\mathbf{curl},\Omega)-$elliptic problems

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Key Words: Auxiliary space preconditioning, IGA, $H(\boldsymbol{curl},\Omega)$, Preconditioning.

Despite the large success of the IsoGeometric Analysis (IGA), dealing with higher-order B-spline functions generate matrices that are denser than the finite element matrices. In general, this leads to a condition number that is not uniformly bounded with respect to discretization parameter h and can even grows rapidly when h goes to zero. As a consequence, the employing of standard numerical solution methods for IGA discrete systems may fail and preconditioning is necessary to obtain convergence in a reasonable amount of time. To overcome the difficulties given by the observed ill-conditioning, in this work we propose the use of what is called the *Auxiliary Space Preconditioning method* [2], ASP method for short, to derive an optimal and robust preconditioning strategy for the linear $H(\boldsymbol{curl},\Omega)$-elliptic problem, on unit square/cube domains, in the case of regular B-Splines finite elements.

From the theoretical side, we have derived a uniform, stable and regular decomposition of the IGA discrete space $V_h(\boldsymbol{curl},\Omega)$, then we have proved the mesh-independent effectivity of the preconditioners by using the abstract theory developed by R. Hiptmair and J. Xu [1]. For the application's part, some sample simulations are developed to test the strategy proposed by our theoretical results in view of further applications. Simulations are conducted on two and three spatial dimensions through three tests. We have first solved the preconditioned linear system, using *Conjugate Gradient (CG)* method, relying on *Jacobi* and on the *Gauss-Seidel* smoothing, then we have investigated the behavior of the preconditioner with respect to the degree refinement, showing in particular that the resulting algorithm can be easily extended to a p-stable algorithm.

The numerical tests show that our preconditioning method has been a very effective cure to the ill-preconditioning of the approximate problem, in the sense that the spectral condition number is sufficiently small and is hardly dependent on the mesh parameter, the number of conjugate gradient iterations necessary to achieve the convergence is essentially independent of the discretization parameter as well as of the B-spline degrees.

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Efficient and Fast Mesh Adaptation Method on more General Geometries using Isogeometric Analysis

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Key Words: Moving Mesh Method, r-Refinemet, Monge-Ampere Equation, Optimal Transport, B-spline, Fast diagonalisation

Adaptive meshes is fundamental for the numerical simulation of the various problems. Thus, the book published by Huang and Russell [1] contains most of the techniques that exist in the literature. However, one that is based on the optimal transport problem is quite powerful because of the guaranteed mathematical properties. Thus, by following the current, we generate a new efficient and accurate sketch of mesh adaptation, especially when we are interested in more general geometries. Hence, inspired by the work of Delzanno et al [2], our idea is based also on the resolution of the Monge-Ampere equation (MAE), but still, in our case, we solve just Poisson equation in each few iterations using the second method introduced by Benamou at al. [3]. Simplifying a lot of computation, we calculate the optimal one-to-one mapping using isogeometric analysis tools to ensure the regularity we need C^1 (or even C^2) and instead of the mesh adaptation on each geometry as presented in the sketch proposed by Delzano et al, which requires a resolution of (MAE) on each deferent geometry, we have simplified this by what we call the inverse image of the adapted mesh on the unit square (single patch domain) and thus always solve (MAE) in the unit square, where the desired adaptive meshes in the physical domain are no other than the image by the initial mapping of this new unit square mesh. From this and using the fast diagonalisation method proposed by Sangalli et all [4] our method is quite really efficient and (fast).

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Immersed Finite Element and Isogeometric Analysis Using Approximate Lagrange Extraction

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Key Words: Immersed Finite Element Analysis, Immersed Isogeometric Analysis, Lagrange Extraction

In this talk, we present a new approach to immersed finite element and isogeometric analysis. In our approach, finite element or spline basis functions defined on a non-body-fitted background mesh are first interpolated onto a Lagrange basis defined on a body-fitted integration mesh, and these background basis function approximations are then employed for immersed finite element or isogeometric analysis. Much like spline basis functions can be represented element-wise in terms of Bernstein shape functions in body-fitted isogeometric analysis [1], the background basis function approximations in our approach can be represented in terms of Lagrange shape functions over each element in the body-fitted integration mesh using Lagrange extraction operators. Consequently, one can transform a classical finite element analysis code into an immersed finite element or isogeometric analysis code with minimal implementation effort using our approach. Namely, one only needs to provide a classical finite element analysis code with Lagrange extraction operators, a connectivity array relating local and global degrees of freedom, and the ability to compute the values and derivatives of the background basis function approximations using the Lagrange extraction operators. In this talk, we will present a stability and convergence theory for our approach for a simple model problem, and we will illustrate the efficacy of our approach using a number of example problems from structural mechanics and fluid dynamics. Finally, we will discuss how we were able to enable immersed finite element analysis within the popular open-source finite element analysis platform FEniCS using our approach [2].

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NURBS Based 2D Curved Bernoulli-Euler Beam Element Using Only Displacement as Variables

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Key Words: *Isogeometric Analysis, NURBS Basis Function, C^{p-1}Continuity, Curved Beam Element, Bernoulli-Euler Beam*

Finite element analysis is widely used for the detailed design of civil engineering structures. However, finite element analysis of curved members has the problem of generating shape errors when we use the non-curved shape elements. Therefore, it is effective to introduce Isogeometric Analysis [1] into the structural analysis of civil engineering structures. This study developed a new two-dimensional curved Bernoulli-Euler beam element using the NURBS basis function. We aim to use our new IGA beam element for the Isogeometric Analysis of thin curved members such as arch ribs and beam string structure.

Several formulations of curved beam elements suitable for IGA have been proposed [2] [3], including the deflection angle as an unknown variable. On the contrary, Weeger et al [4] developed a nonlinear Bernoulli-Euler beam element using only displacements as an unknown variable. In the article, they focused on the spline functions that can automatically maintain continuity of deflection angles between elements. Therefore, we also developed a curved Bernoulli-Euler beam element with only displacement as an unknown variable.

In the present study, we adapted the definition of strain based on the theory of two-dimensional curved Bernoulli-Euler beams [5] and discretized using a finite element method based on the Galerkin method. The trial function consisted of a linear combination of NURBS basis functions and displacement on each control point. Finally, we found that the convergence rate of the relative error to the exact solution decreased with decreasing element length. Furthermore, we evaluated the proposed curved elements with varying curvatures. As a result, our proposed element could solve any curved beams with high accuracy.

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Stabilized Isogeometric Discretization of the Navier-Stokes-Korteweg Equations: Toward Predictive Cavitation Simulations

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Key Words: *Cavitation, Stabilized formulation, Isogeometric Analysis, Navier-Stokes-Korteweg*

Cavitating flows are ubiquitous in engineering and science applications. Despite their significance, a number of fundamental problems remain open; and our ability to make quantitative predictions is very limited. The Navier-Stokes-Korteweg equations constitute a fundamental model of cavitation [1], which has potential for predictive computations of liquid-vapor flows, including cavitation inception —one of the most elusive aspects of cavitation. However, numerical simulation of the Navier-Stokes-Korteweg equations is very challenging, and state of the art simulations are limited to very small Reynolds numbers, open flows (no walls), and in most cases, micrometer length scales [2-3]. The computational challenges emerge from, at least, (a) the presence of third-order derivatives in the governing equations, (b) a complicated eigenstructure of the spatial partial-differential operators in the governing equations, which prevents the use of standard finite volume techniques, and (c) the need to resolve the liquid-vapor interface, which without special treatment, has a thickness in the order of nanometers. Here, we present a stabilized isogeometric discretization scheme that permits, for the first time as far as we are aware, large-scale simulations of wall-bounded flows with large Reynolds numbers. The proposed stabilization scheme is a residual-based approach that emanates from the eigenstructure of the equations and vastly outperforms standard stabilization schemes for advection-dominated problems. We feel that this work opens possibilities for predictive simulations of cavitation.

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A new numerical iterative method for calculating the load capacity of truss constructions

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Key Words: *truss constructions, stick direction coefficient, Ritter-Križaić iteration method, algorithm truss Mathcad*

Optimization of the dimensioning of structural structures is gaining momentum. FEM, evolutionary, and other methods are found that are transformed by algorithms into computer simulations of construction models. Using existing methods and interconnecting and merging these structures yields a new, seemingly complicated, but simple method that computers can easily support with software loops. By setting the geometric characteristics of constructive lattice systems in equation lines, formulas are obtained that replace even trigonometric equations. The Ritter-Križaić iterative method for one-sided gratings with a flat lower band is also defined. This method paves the way for new methods to define different types of grids. By solving demanding models, i.e., by defining an iterative model with oblique rod belts sticks, the definition of spatial variables necessary for static dimensioning of structures is accelerated. As a result, the approach of simple n-polygonal structural modeling of truss continuous construction with combination direction coefficients and defining differential equations of a grid's continuum in displacement with the Mathcad toolset is developed.

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Calibration and Validation of DEM and CFD-DEM Models of Industry-Relevant Systems using Evolutionary Optimisation and Positron Emission Particle Tracking

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Key Words: *Discrete Element Method, Industrial Applications, Calibration, Validation*

The discrete element method (DEM) is a powerful tool capable of predicting the dynamics of diverse particulate systems with quantitative accuracy. However, if not correctly calibrated, the results of DEM simulations can be inaccurate or even unphysical. As such, the calibration and validation of DEM simulations is an important task, but one which carries significant complexity. In particular:

1. DEM models require details of *microscopic* quantities (sliding and rolling friction coefficients, restiution coefficients...), but conventional powder characterisation measure only *macroscopic* quantities (internal friction angle, yield stress...) making the rigorous determination of accurate calibration values highly challenging.
2. The meaningful validation of DEM models requires the detailed, multi-point comparison with experimental results. As many industrial systems are metal-clad and thus optically-opaque, the use of common imaging techniques such as PIV is precluded.

In this talk, we detail solutions to both of these challenges developed at the University of Birmingham. Regarding the former, we briefly introduce the recently-developed ACCES (Autonomous Characterisation and Calibration using Evolutionary Simulation) technique which uses evolutionary algorithms to backcalculate the microscopic parameters of particulate media from measurements of their bulk behaviours. Regarding the latter, we discuss how Positron Emission Particle Tracking, a technique capable of extracting high-resolution, three-dimensional data from optically-opaque systems, may be leveraged to provide rigorous, detailed validation of DEM and coupled CFD-DEM simulations of industry-relevant systems.

Modelling of keyhole dynamics and melt pool flow in selective laser melting additive manufacturing

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Key Words: *selective laser melting, additive manufacturing, keyhole, fluctuation, melt pool flow, recoil pressure*

As one of the promising additive manufacturing (AM) technologies, selective laser melting (SLM) fabricates metal components layer-upon-layer using laser beams to fuse metallic powder. The keyhole is produced commonly at high energy density (high laser power or low scanning speed) during the SLM process. However, the dynamics of keyhole and melt pool, and their relationship with forces remain unclear. Here, through the developed three-phase volume of fluid (VOF) model [1], the quasi-stable keyhole dynamics and metal powder melting process are captured. Results show that the keyhole life cycle experiences steps of formation and drilling, fluctuation, and disappearance. Pores are generated from the gas void in the powder bed, keyhole protrusion, and the end eroded gas bubbles. During the laser-on period, an anticlockwise vortex is generated at the tail, and the liquid travels in a clockwise path ahead of the melt pool. The stability of the keyhole depth is disturbed by the powder layer thickness variation, and it oscillates repeatedly until the laser is off. The centrifugal flow at the tail body of the melt pool is driven at the combined action the surface tension and Marangoni force. The rear keyhole is compressed dominated by the surface tension while the front rim is expanded controlled by the recoil pressure. The present study enhances the further understanding of multi-physics in SLM process.

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Numerical analysis of debris-like flow using an extended CFD-DEM method based on micropolar fluids

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Key Words: *Micropolar fluids, discrete particle, debris-like flow, micropolar parameters*

Debris flow, a multiphase system containing multi-scale particles, often occurs in geological hazard, causing serious economic losses and casualties. Therefore, it is important to deeply understand the mechanism of the debris flow and establish an effective scheme to monitor and prevent its large-scale occurrence. But, researches on the occurrence and movement of the debris flow is difficult to be carried out by experiment due to the complexity of geological conditions. Thus, numerical simulation could be a main approach to predict the movement of the debris flow, and the selection of mathematical model for describing the debris flow movement is the guarantee of the effectiveness of the simulation. In this study, based on the physical mechanism of microstructure effect considered in the micropolar fluids model [1], and its application in suspension system [2]. We established a coupling computation model (MVD model) considering the micropolar fluids to describe the mixed system with small particles and VOF (volume of fluid) method to track the free surface of liquid and discrete element method (DEM) to describe the movement of larger particles and their interaction. The main works include (1) the solution and verification of the MVD model under single particle sedimentation test [3], (2) the comparison of the debris-like flow morphology with DEM, classical fluid-particle coupling model and MVD model, (3) the analysis of the debris-like flow under different micropolar parameters, particle volume fraction, particle size distribution and slope gradient based on the MVD model. Numerical results indicate that the fluid with microstructure plays a significant role in the occurrence and movement of the debris-like flow and other factors have a certain effect on the movement characteristics of the debris-like flow.

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On modeling of large particle size variations in DEM-CFD simulation

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Key Words: *DEM-CFD Method, Signed Distance Function, Immersed Boundary Method*

A solid-fluid multiphase flow including large particle size variations is ubiquitous in industries. In this system, large sized objects and small sized particles are mixed. Since understanding of the large particle size variations is not sufficient, application of numerical model is desired. In the present study, we develop a new model to simulate the large sized object which is mixed with small sized particles. In this model, the contact force is simulated by the linear spring model and the drag force is computed by combination of the signed distance function (SDF) [1] with the immersed boundary method (IBM) [2]. The small sized particle is calculated by the discrete element method (DEM) [3]. The new model is incorporated into our in-house code which is referred to as FELMI [4]. In order to show adequacy of the new model, we perform a validation test. In the validation test, we employ the fluidized bed system, where a large sized object is mixed with the small sized particles. Herein, the object position is compared between the computational and experimental results after fluidization is terminated. The large-sized object position well agreed between the computation and the experiment. Hence, Adequacy of the new model is proved through the validation test.

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Study on rolling resistance model of discrete element method based on material elastic hysteresis theory

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Key Words: *Granular material; Rolling resistance; Elastic hysteresis; Speed independent; Discrete element*

In this paper, the mechanism of particles' rolling resistance caused by elastic hysteresis in collapsing elastic granular materials is studied at the meso-scale. A rolling resistance model applicable to the discrete element method is proposed.

Firstly, we analyze the rolling resistance behavior due to the material's elastic hysteresis during the rolling process of an elastic, round particle under different compression and relaxation pressures at the front and rear areas of the contact surface. Subsequently, the mechanical model of rolling resistance caused by material elastic hysteresis is established.

Then, the particle material's elastic hysteresis constitutive curve under compression (loading)and relaxation pressures (unloading) is measured by experimental method. The particle material's elastic hysteresis parameters are obtained, and a formula of particle rolling resistance for the discrete element method is proposed.

Finally, the formula is applied to the discrete element model to simulate the rolling process of an elastic circular particle on a rigid surface, and the simulation results are verified by a physical experiment. The results show that the rolling resistance model based on the material elastic hysteresis theory can effectively reproduce the rolling resistance behavior of elastic particles in granular materials.

Adaptive Computations for Biot System Based on A Posteriori Error Estimate with Mixed Finite Element Method for Flow

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Key Words: *Error Estimate, Mixed Finite Element Method, Biot System, Iterative coupling*

Coupling Geomechanics to flow has greatly improved the accuracy of subsurface modeling. In this paper, we present an adaptive mesh refinement and iteration stopping algorithm based on a posteriori error estimates for solving the Biot system. The mechanics system is approximated by conforming Galerkin method (CG) while the flow is solved by mixed finite element method.

The Biot system commonly appears in geosciences and biosciences for modeling carbon sequestration (Lu and Wheeler 2020) and tissue deformation during subcutaneous injection (Leng, Lucio and Gomez 2021). Previous works have indicated that ensuring local mass conservation for the flow (Choo and Lee 2018) is crucial to the accuracy of the simulation, making Enriched Galerkin (EG) (Girault, Lu and Wheeler 2020) and mixed finite element method attractive options. Here we restrict our work to solving the flow with mixed finite element method and fixed-stress split for resolving the Biot system. A posteriori error estimates are derived for such algorithm to quantify different error components. The error estimators provide a novel adaptive stopping criterion, which balances algorithmic error from fixed-stress split and discretization error in space and time, for the fixed-stress iterations. We also demonstrate adaptive mesh refinement guided by the error estimators for simulating fractured reservoirs.

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15th World Congress on Computational Mechanics (WCCM-XV)
8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII)
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Efficient Implicit-Explicit Time Integration for Multiscale Simulations Using Hybridized Finite Element Methods

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Key Words: Multiscale methods, multinumerics, hybridized finite elements, time integration methods

Hybridized finite element methods have grown in popularity over the past 20 years, primarily for implicit time integration schemes with higher-order spatial discretization because the global linear system is much smaller than that of comparable methods. In addition, hybridized methods can be derived as variational multiscale methods [1], but have additional benefits due to the flexibility provided by the mortar grid. This perspective is well-suited for multiphysics problems and naturally allows for different resolutions and numerics throughout the computational domain [2]. For hybridized methods, the decomposition can be pushed to the element level, effectively providing such flexibility at the element-by-element level.

Recently, there has also been an interest in developing explicit and implicit-explicit (IMEX) methods to bolster the applicability of hybridized methods [3, 4, 5]. For wave propagation applications, explicit methods are attractive when the timestep required for stability is similar to that required for accuracy. However, for many practical problems, subgrid scale physical features in the medium render explicit integration prohibitively expensive; therefore, IMEX schemes based on domain decomposition become an attractive alternative. In this work, we explore the stability, accuracy, and performance of generalized IMEX methods for hybridized finite element methods in massively parallel computational environments. We will include applications in shallow water and wave propagation through heterogeneous media.

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Multiscale and Multiphysics modeling of Cardiac Hemodynamics

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Key Words: Heart Modeling, Multiphysics Problems, Computational Fluid Dynamics, Variational Multiscale Methods, Large Eddy Simulation, Stabilization Methods

Computer-based numerical simulations of the heart and blood circulation represent a valuable tool to analyze the cardiac function and to enhance the understanding of cardiovascular diseases. In this talk, we introduce a Computational Fluid Dynamics (CFD) model for the numerical simulation of the whole heart hemodynamics, by accounting for all the physical processes that influence cardiac flows: moving domain and interaction with electromechanics, transitional-turbulent flows, cardiac valves and coupling with the external circulation. We employ the Navier-Stokes (NS) equations in Arbitrary Lagrangian Eulerian (ALE) framework and the Resistive Immersed Implicit Surface (RIIS) method to model the presence of valves in fluid. To impose a physiological displacement of the domain boundary, we employ a cardiac electromechanical model obtaining thus a multiphysics one-way coupled electromechanics-fluid dynamics model [1]. To better match the 3D CFD with blood circulation, we also couple the 3D NS equations to a 0D closed-loop circulation model. We obtain a multiphysics and multiscale coupled 3D-0D fluid dynamics model that we solve via a segregated numerical scheme [1]. We use a Variational Multiscale - Large Eddy Simulation (VMS-LES) method [2] to get a stable formulation of the NS-ALE-RIIS equations discretized by means of FE Method, to stabilize the advection-dominated regime, and to account for turbulence modeling within the framework of LES. Finally, we propose the ehnancement of residual-based stabilization methods via Artificial Neural Newtorks (ANNs). By considering numerical tests for the simpler case of advection-diffusion PDEs with SUPG stabilization method, we show that our ANN approach yields more accurate solution than using the conventional SUPG method [3].

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Simple Models for Linear and Singular Losses for Periodic Flow

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Key Words: Finite element methods, hydraulic losses in periodic flow

Many attention has been paid to the losses in pipes and singular elements of fluid systems for stationary flow [1]. However, some systems found in engineering, biology and nature are based on pulsatile flow and/or periodic flow. This is the case of the circulatory system or the design and testing of dampers based on hydraulic circuits. In this work, based on the theory of dynamical systems, dimensional analysis and computational fluid dynamics, a simple model for the losses of various elements as a function of frequency is developed [2,3].

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Streamline-Upwind Petrov-Galerkin formulation for the analysis of hypersonic flows in thermal non-equilibrium

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Key Words: *Compressible flows, Stabilized methods, Shock capturing, Finite elements, Reacting flows, Thermal non-equilibrium, Hypersonic flows*

This work presents a Streamline-Upwind Petrov-Galerkin (SUPG) framework with finite elements discretization for the prediction of non-ionized hypersonic flows in thermal non-equilibrium. The formulation is enhanced with a residual based discontinuity capturing (DC) operator. The numerical framework solves the set of Navier-Stokes equations for the compressible reacting flows with an additional equation for the vibrational-electronic energy conservation. The set of equations, which involves one continuity equation for each chemical species considered, is solved in the pressure-primitive variables. The framework was recently validated for the non-reacting hypersonic flow problems in [1]. The numerical framework capabilities are assessed through several benchmark cases, including validation of the chemical model and its coupling with the two temperatures model in the context of critical flow features such as shock-shock and shock-wave boundary layer interactions. The first test case presented is 0D nitrogen reactor case which is a transient evolution of reacting nitrogen in vibrational non-equilibrium. The next case is the 2D cylinder case immersed in a Mach 12.7 flow of a 5-species reacting air mixture in thermal non-equilibrium. The last two cases are the 3D axisymmetric hollow cylinder extended flare (HCEF) and the double cone. Detailed measurements of the surface pressure and heat flux for the HCEF and the double cone in high-enthalpy flows have been obtained during a series of experiments carried out in the LENS XX expansion tunnel facility. The accuracy of the results is assessed through the comparison with the numerical and experimental data available in the literature for all the test cases presented. The numerical results demonstrate the suitability of the formulation in predicting non-ionized reacting hypersonic flows in thermal non-equilibrium.

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Variational-Multiscale Discontinuous-Galerkin Method: Application to Additive Manufacturing

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Abstract

This talk presents mathematical constructs underlying the Variational Multiscale Discontinuous Galerkin (VMDG) method [1,2,3]. It results in a robust finite element approach for mathematical problems with weak and strong discontinuities, and also facilitates a unified framework to derive interface transmission conditions. The method accommodates non-matching discretizations and optimal error convergence rates are presented.

The method is applied to extrusion-based layered printing with cementitious materials [4]. The evolution of mechanical properties as the printed material cures and stiffens results in non-physical reduction in the magnitude of elastic strains when standard constitutive models are employed. This elastic recovery of the printing induced deformation contradicts the experimentally observed behavior of the printed cementitious materials that harden at a nearly-frozen deformed state. A thermodynamically motivated constraint on the evolution of elastic strains is imposed on the constitutive model to remedy the non-physical bounce-back effect. An algorithm that is based on a strain-projection technique for the elastic part of deformation is developed that complements the inelastic response given by the Drucker-Prager model A ghost mesh method is proposed for continuous layer-wise printing of the material without the need for intermittent mesh generation technique or adaptive remeshing methods. The model is validated via comparison with experimental data and representative test cases are presented that investigate the mathematical and computational attributes of the proposed model.

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A fluid-thermal multi-physical field simulation model for proton exchange membrane fuel cell

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Key Words: *fuel cell, heat transfer simulation, water management*

Hydrogen is a secondary clean energy for sustainable development, and fuel cell is the main way to use hydrogen energy [1]. Proton exchange membrane fuel cell (PEMFC) directly converts the chemical energy of hydrogen into electrical energy through electrochemical reaction, which avoids the limitation of Carnot cycle and has a huge market prospect.

Water will be produced during the operation of oxyhydrogen fuel cells. The accumulation of water will accelerate carbon corrosion and reduce the performance of the battery [2]. On the other hand, if the fuel cell is dry for a long time, the proton exchange membrane fuel cell will dry and break, which will also cause damage to the fuel cell [3]. The temperature distribution of the battery has a great influence on the output power and indirectly affects the water content [4]. Uneven temperature distribution will lead to serious degradation of the membrane and catalyst layer, thus shortening the battery life [5]. The coupling relationship between water and heat management can not be ignored.

In this study, COMSOL was used to establish the simulation model of proton exchange membrane fuel cell, and the heat and mass transfer process in the cell was coupled with electrochemistry. The results show that by simulating the real-time state of the battery and adjusting the parameters, the irreversible damage to the battery can be avoided and the battery life can be effectively prolonged.

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A neural network-based SIMPLE algorithm for large-scale fluid simulation

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Key Words: *Pressure Poisson equation, Deep neural network, Deep Residual Iteration Method, Fluid simulation*

In the SIMPLE algorithm for incompressible flows, solving the pressure Poisson equation is usually one of the key steps with the longest time consumption. In this study, a method based on deep neural network is proposed to accelerate this process: first, the equation is transformed into multiple independent tridiagonal subproblems based on the Fast Fourier Transform, and the subproblems are solved in fast parallel using a deep residual network. For the problem with more than 100,000 grids, this optimized SIMPLE algorithm has more than 10 times efficiency improvement in GPU platform compared to traditional methods. In addition, the algorithm effectively overcomes the shortcomings of neural networks in terms of interpretability and accuracy compared to other neural network methods, and has high numerical accuracy in typical cases such as driven cavity flow and backstep flow, and provides a promising means of implementation for large-scale direct numerical simulation.

BDD Preconditioner for A Diagonal-scaled Schur Complement System

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Key Words: *Balancing Domain Decomposition, Non-overlapping Domain Decomposition, Schur Complement, Diagonal-scaling Preconditioner*

Many of actual problems in science and engineering fields have multiple different materials and are modelled with large-scale unstructured mesh. The Domain Decomposition Method (DDM) based on the iterative methods is well-known as an effective parallel finite element method, however, solving such problems will suffer from slow convergence rate or no convergence. In order to achieve high performance in both convergence rate and parallel efficiency, it is necessary to apply an effective preconditioner for the DDM.

The Balancing Domain Decomposition (BDD) preconditioner [1] is an effective preconditioner for its very fast convergence rate. However, in considering composition of very different materials for actual problems, the convergence rate of the BDD is also shown to be worse. Some studies extended the BDD preconditioner to such problems with jumps in coefficients [2][3], but these are not suitable for cases of complex shape and composite materials. On the other hand, some numerical experiments show that a BDD-DIAG method [4], which uses a diagonal-scaling preconditioner instead of the Neumann-Neumann one, has robust convergence for the multi-materials.

In this study, to accelerate convergence of BDD preconditioner for the multi-materials, a BDD method combined with diagonal scaling preconditioner is considered and some numerical examples are demonstrated.

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Derivation and Validation of Compressible PTT Viscoelastic Fluid Model

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Key Words: *Viscoelastic Model, PTT, Network Theory, Planar Poiseuille Flow*

A number of investigations of linear or nonlinear viscoelastic fluid models have been proposed. Examples are Upper-Convected-Maxwell fluid model [1], Oldroyd-B model [2], Giesekus model, FENE model and many others. A new viscoelastic model among these is the Phan-Thien–Tanner (PTT) model for which one can reasonably hope to obtain the analytical and numerical solutions. The constitutive equation of the PTT model was derived using network theory [3,4]. This model has advantages over others because it includes not only shear viscosity and normal-stress differences but also an elongational parameter ε. Therefore it reproduces many features of the rheology of polymer solutions and non-Newtonian liquids.

Micro-macro models of polymeric viscoelastic fluids that arise from statistical physics are based on coupling Navier-Stokes system to conservation equation of network theory. In the model polymer molecules are idealized as linear or unbranched chains, connected by junctions to constrain chains so that the connected points move together for at least a certain minimum length of time. Network is formed by a set of chains connected by junctions such that every junction is linked by at least one unbroken macro-molecular path to a boundary point.

This research derives a new PTT model for compressible fluids. The elastic extra stress tensor $\mathbf{T}$ and polymer density η are contained in the governing equations derived from polymer network theory and combined with compressible Navier-Stokes equations the non-Newtonian elastic extra stress tensor is rederived. Planar Poiseuille flow is simulated based on the compressible PTT model and the accuracy of model is validated by numerical results compared with the analytical results.

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FE Analysis of Numerical Human Body Model with 100 Million DOFs in High-Frequency Electromagnetic Field - Heat Conduction Coupled Problem

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Key Words: *High-Frequency Electromagnetic Field - Heat Conduction Coupled Analysis, Parallel Computing, Finite Element Method, Hierarchical Domain Decomposition Method, Human Body Model*

In order to evaluate an effect of cancer treatment by hyperthermia quantitatively, we have been studying its high-frequency electromagnetic field – heat conduction coupled analysis in a parallel environment. In our study, the NICT numerical human body model [1] is analyzed. This model uses a binary data format wherein types of organs are encoded using voxels. The diameters of cancers treated with hyperthermia are several millimeters; thus, elements must be refined to obtain sufficient accuracy. However, there are approximately 1 trillion degrees of freedom (DOFs) provided that the element sizes are 0.1 mm. In addition, smoothing techniques to reduce numerical noise increase the DOFs further. The efficient parallel computing method for large-scale finite element analysis (FEA) that we have been studying is the iterative substructuring method in the form known as the domain decomposition method (DDM) based on the iterative method [2]. It is expected to obtain scalable parallel efficiency on distributed memory parallel computers with the implementation of a Hierarchical Domain Decomposition Method (HDDM) [3]. The HDDM has been applied to the large-scale FEA of electromagnetics, and high-frequency electromagnetic field problems have been solved with 130 billion DOFs [4]. As the next step, a parallel coupled analysis is considered. In this presentation, the numerical human body model involving 220 million DOFs is analyzed in the parallel environment.

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High-performance Parallel Smoothed Particle Hydrodynamics Solver Based on Multi-section Division and Hashed Tree Method

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Key Words: *Smoothed Particle Hydrodynamics; Numerical analysis; Computational fluids dynamics; Domain decomposition; Multi-section division; Fast neighbor search; Hashed-Tree method; High-performance parallel computing;*

As a new generation of CFD scheme for complex hydrodynamics problems, the SPH (Smoothed Particle Hydrodynamics) numerical method was developed in the late 1970s. After being subsequently tailored to the modelling of elastic media, particularly for the calculation of the very large strains and the fracture phenomenon, it was repeatedly improved before being applied, as of the early 1990s, first to weakly compressible hydrodynamics, then to strongly compressible[1] and truly incompressible[2] hydrodynamics.

As an interpolation method, the accuracy of the SPH method often depends on the number of particles in the support domain. In theory, when the number of particles approaches infinity, the computational accuracy will be very close to reality. However, as an adaptive method, SPH has to run a large amount of computation at each time step, which is quite time-consuming and limit the development of the method[3].

This paper reports our high-performance smoothed particles hydrodynamics solver on distributed parallel computational system. In the solver, a highly efficient domain decomposition method based on multi-section division and the sampling method was proposed which could make the distributed computing system achieve load balancing with negligible work. For the search for neighbouring particles, an algorithm called Hashed-Tree Method was implemented to accelerate the initialization of the hierarchical data structure with well parallelization. The actual performance of the solver was assessed in detail through numerical simulations at various scales. Not only the weak scaling performance could be almost linear speed up but also high efficiency is achieved for strong scaling tests.

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Implementation of Balancing Domain Decomposition Method for Inactive Elements and Its Applications

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Key Words: Parallel Finite Element Method, Domain Decomposition Method, Inactive Element Method, Damage Analysis, Additive Manufacturing Analysis

The domain decomposition (DD) method is a powerful parallel computing technique for finite element analysis of solid mechanics problems at large scales. Although various DD methods have been proposed so far, the present study uses the balancing domain decomposition (BDD) method [1] and the BDD with diagonal scaling (BDD-DIAG) method [2].

In the DD methods, the analysis model should be decomposed into subdomains for parallel computing, before the linear system of equations is solved. In many solid mechanics problems, the analysis model does not change throughout the analysis with time steps. This means that the analysis model is decomposed only once at the beginning of the analysis. However, in some problems such as severely large-deformation problems, crack propagation problems and machining problems, regeneration of the domain-decomposed analysis model is necessary at every time step or every few time steps.

Furthermore, one can find another type of problem that is the focus of the present study. In this type, the analysis model involves inactive elements that are finite elements having zero stiffness. For example, multi-pass welding analysis and additive manufacturing analysis use the inactive elements to model the region to be solidified. Moreover, in damage analysis, the inactive elements can be found when the damage variables reach unity. For these problems, we adopted the one-time decomposition approach, in which the DD process is performed once at the beginning of the analysis. To adopt this approach, we need to formulate an implementation method to constrain floating degrees of freedom caused by the inactive elements.

In the present study, we present an implementation method for the BDD and BDD-DIAG solvers with the inactive elements. Moreover, its applications to damage analysis and/or metal additive manufacturing analysis will be demonstrated in the presentation.

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Numerical Integration Technique Using Background Cells for Weak Form Constraint Condition of Dual Lagrange Multiplier Method

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Key Words: *Assembly Structure, Mortar Finite Element Method, Balancing Domain Decomposition Method, Dual Lagrange Multiplier, Multipoint Constraints, Weak Form, Background Cell*

Incorporation of a set of linear multipoint constraints (MPCs) in finite element analysis is important for performing realistic structural simulations. Miyamura[1] proposed a method to incorporate MPCs into the balancing domain decomposition (BDD) method (BDD-MPC method).

In the mortar finite element method, constraints to connect structural components are imposed in a weak form with a surface integration. The constraints can be represented by Lagrange multipliers that are interpolated using a set of shape functions. In the dual Lagrange multiplier method[2], the Lagrange multiplier is interpolated using a set of biorthogonal shape functions. After the surface integration for the constraints is conducted, a constraint matrix with respect to nodal displacements is obtained, that is, the constraints in a weak form are represented as a set of MPCs. In general, mesh patterns of two surface patches of two meshes to be connected are inconsistent. Sando et al.[3] proposed a method that uses integral cells generated by triangulation on the constraint surfaces for the integration of the weak form. In this study, the Gauss integration is performed in square cells called background cells, which are arranged in a grid pattern. The pattern is independent of the mesh patterns of two patches to be connected.

Examples of simple assembly structures whose constraint conditions in weak form can be integrated using only one cell were presented in the previous study[4]. In this study, examples of constraint conditions that are integrated using multiple cells are shown. The analyses are performed using the BDD-MPC method, and the convergence properties of the method are also investigated.

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Positive-Definiteness of the Coarse Matrix in BDD-DIAG of a Perturbed Maganetostatic Problem

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Key Words: *Large Scale Magnetostatic Problems, Preconditioning, The Coarse Problem*

Until now, we have considered the Balancing Domain Decomposition DIAGonal scaling (BDD-DIAG) preconditioner as a preconditioner of non-overlapping domain decomposition analysis of 3-dimensional magnetostatic problems taking the magnetic vector potential as an unknown function. One interesting fact is that the direct solver can be used in many cases for solving the coarse problem in BDD-DIAG. In this paper, we show a sufficient condition for positive-definiteness of the coarse matrix in BDD-DIAG of a perturbed maganetostatic problem. Though our numerical results are got in many cases of the original magnetostatic problem, we mainly consider the well-known perturbed problem in this paper. A conjecture is also given for the original magnetostatic problem.

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A real-time data-driven modelling frawork for control and simulate the behavior of industrial controllers

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Key Words: *Machine learning, real-time control, neural network, stable integrators, data-driven*

Online control and prediction of controller behaviour is often a tricky issue, especially when it comes to sensitive tasks requiring control within few milliseconds. Previous works used dynamic mode decomposition approach (DMD) to build a digital twin, learning therefore a stable correction and integrator of the controller [1]. Moreover, regularization is used to train a stable time integrator using DMD method.

On the other hand, DMD can be extended to nonlinear settings, where DMD is trained locally, which leads to the need of training multiple local integrators and then select the most appropriate in operation depending on the location in the phase space.

In this work, we train a non-linear integrator, using machine learning techniques and recurrent neural networks. Multiple models are trained and used in this work. The result is first a real-time controller behaviour prediction in fraction of milliseconds. Second, a stable real-time integrator is trained to perform real-time controller simulations. Both models are tested against data sets never used in the training.

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Complexity Reduction of Geometrically Parametrised Turbulent Flows via Reduced Order Models.

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Key Words: Reduced Order Models, CFD, Turbulence, Industrial Applications

The complexity associated with geometrically parametrised flow problems represents a limitation to the application of conventional, or high-fidelity, techniques. On the other hand, on such applications reduced order models (ROM) show great potential, allowing for the efficient solution of complex systems. This work presents a hybrid strategy to build a reduced model applicable in industrially-relevant applications. The methodology combines data-driven and projection-based techniques. It consists of constructing the reduced basis by means of the well-established proper orthogonal decomposition (POD) [1], and a Galerkin projection of the Navier-Stokes problem for the evaluation of the parametric coefficients. The eddy viscosity, and in effect the turbulent contribution is approximated via an interpolation scheme, i.e. POD-I, significantly improving the versatility of the methodology.

Aiming towards industrial applications, this work considers the most commonly-employed methodologies, i.e. the Finite-Volume Method (FVM) and the Reynolds-Averaged Navier-Stokes equations (RANS). For improved implementation, the sampling procedure and the calculation of the reduced operators in the offline phase use OpenFOAM's [2] open-source libraries, while the data separation and the online problem are solved using Python.

Finally, the capabilities of the proposed strategy are tested by approximating the turbulent flow around a NACA aerofoil with parametrised angle of attack, expanding the work presented in [3] to turbulent problems.

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Extraction of Implicit Knowledge and Optimization

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Key Words: Dimensionality reduction, Topological and geometrical characterization, Interpolation, Optimization

Those last years have seen a growing maturity in optimization tools, particularly topological optimization [1]. Nevertheless, those methods do not take the accumulated knowledge of industrial manufacturers into account. Moreover, they face substantial limitations to include all the various constraints that govern the realization of industrial products.

We wish to ally discovery tools from IA and optimization ones in this project. A key question is that the amount of design of a given industry is very low and thus it is not possible to use deep-learning approaches for this purpose. Therefore, among the possible tools we have elected those allowing to infer, if possible, a reduced manifold of the existing design. If the latter is of low dimension optimization my then be performed in this manifold. The second question is what type of descriptors and classification are the most appropriate to perform the dimension reduction and to interpolate properly within the existing design. Those tools combine reduced modelling and manifold learning approaches (like Locally Linear Embedding) [1], geometrical characterization (Level set [2]), Topological Data Characterization [3] and optimal transport [4]. Those tools are today of easy access through dedicated libraries.

Those basic concepts will be illustrated with 2D examples mimicking bumpers. At the present stage, it seems that we are capable of defining the geometrical manifold of bumpers and interpolate following the manifold. We are looking to incorporate mechanical information such as von Mises maps to enrich the description of the manifold.

Our present focus, which we hope to be able to illustrate during the conference, is to make use of the enriched manifold to be able to optimize along the variety of "validated design', that is, to create know-how optimization tools.

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Finite Element Method Based Neural Network for Forward and Inverse problems

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Key Words: *Finite Element Method, Digital Twin, Informed Machine Learning, Hybrid model*

A hybrid model combining the Finite element method (FEM) and neural network is introduced for forward and inverse problems. The model uses the discretized form of the governing equation as the loss function of the neural network. As mentioned above, the requirement for the target variable for the neural network's training is avoided, resulting in an unsupervised learning approach. The hybrid model falls in informed machine learning [1] and introduces a new direction to combine FEM and neural network.

The proposed hybrid model can create a surrogate model for forward solving of Partial Differential Equations. The FEM will provide the discretized system matrix and force vector, whereas the neural network predicts the solution vector. The matrices, along with the prediction, are used inside the loss function of the neural network. The calculated loss is backpropagated through the neural network to optimize the network parameters. A digital twin can use such trained networks for real-time simulation.

The same algorithm can be used for inverse problems as well. The unknown parameters are modeled using a neural network and assembled to the system matrix using FEM principles. Using the measured response and known forces, a similar loss function as that for the forward problem is formulated and backpropagated to optimize the parameters of the neural network. The trained neural network can then be used as the model for unknown parameters of the model.

Both the forward and inverse problems are demonstrated with the examples. Forward solving is demonstrated for the wind load on a high-rise building [2]. The application of the surrogate model is shown with the help of an uncertainty quantification problem using the Monte-Carlo method.

The inverse problem is demonstrated in finding the bearing parameters of fluid bearing in a rotor dynamics problem. The speed-dependent stiffness coefficients of the fluid bearing are modeled using a neural network and trained using the vibration measurement and known unbalance in the test rig.

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Learning physics with metriplectic and geometric biases

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Key Words: Geometric Deep Learning, Structure-Preserving Neural Networks, GENERIC

Deep learning-based artificial intelligence success in computer science has encouraged many authors to transfer this new technology to the physical simulation field. The challenging task of those research lines is to adapt state-of-the-art deep learning tools into physics and engineering, two disciplines with centuries of experimental and theoretical background. In our work, we develop a deep learning framework to predict the evolution of complex physical systems using that knowledge in a form of several inductive biases, which guide the learning algorithm to find the physically consistent target function.

The first inductive bias enforces the metriplectic structure of dissipative dynamics via the GENERIC formalism [1]. This formulation imposes the physical consistency by using thermodynamics, describing the system as a sum of a conservative term (related to conservative energy and Hamiltonian mechanics) and a dissipative term (related to entropy and the irreversible physics of the system). Furthermore, the degeneracy conditions of this formulation ensure the energy conservation and the entropy inequality, fulfilling the first and second laws of thermodynamics respectively.

Learning this specific mathematical structure is a challenging task for a standard neural network, as physical systems may have complex local interactions based on geometrical constraints. Thus, we develop a graph-based architecture to take advantage of the structured mesh information and make computations over the topology of the domain [2]. The use of geometric deep learning is also convenient for introducing symmetries to the problem, such as permutation or translational invariance, which decrease the data consumption of the method. The combined use of the metriplectic and geometric bias is tested with several nonlinear examples of solid and fluid mechanics.

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On the GENERIC formalism and its role in learning physics from data

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Key Words: Scientific machine learning, dissipative systems, inductive biases, GENERIC.

Soon after the widespread interest in applying deep learning technology to the field of computational mechanics appeared, our community has realized that it is of utmost importance to enforce the fulfillment of physical laws to guarantee that the obtained predictions comply to the physical reality. In general, this is done through the employ of inductive biases of various types.

In some of our previous works [1, 2] we have employed the enforcement of the metriplectic structure of dissipative problems through the so-called GENERIC formalism [3]. Using GENERIC as an inductive bias ensures the satisfaction of the first and second principles of thermodynamics (conservation of energy in closed systems and non-negative entropy production, respectively). This enforcement is done in a soft way in our works, although recent approaches to the same problem have chosen to do it in a hard way [4, 5].

In this work we will discuss about the statistical mechanics of machine learning, the implications of choosing GENERIC as the inductive bias and the appealing of the results it gives.

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Surrogate modeling with proper orthogonal decomposition for predicting electrochemical potential distributions in SOFC

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Key Words: Surrogate model, Proper orthogonal decomposition, Numerical simulations, Solid oxide fuel cell, Electrochemical potential

The capability of solid oxide fuel cell (SOFC), which generates electricity using hydrogen as a fuel, is determined by not only the electrochemical performance but also the mechanical durability, for which predicting the transient nature of the electrochemical potentials is of paramount importance. To this end, Terada et al.[1] and Muramatsu et al.[2] proposed the numerical analysis method to evaluate the time-varying electrochemical potential distributions under various start-and-stop control environments. However, due to the highly nonlinear behavior such as the environment-dependent physical properties, fairly fine time step should be taken to stably obtain the results with high accuracy.

To overcome this issue, we propose a method of surrogate modeling with proper orthogonal decomposition (POD) that is capable of predicting the non-stationary distributions of electrochemical potentials in an efficient way. First, a series of *offline* numerical analysis is carried out under various target conditions taken, e.g., for design purposes. Second, POD is applied to the obtained data matrix that stores all the results following certain rule of thumb to represent each simulation result by a linear combination multiplied by the corresponding coefficients. Third, the coefficients are interpolated within the parameter space specifying the prepared analysis conditions to construct the surrogate model that enables us to realize *online* numerical analysis under an arbitrary condition. A representative numerical example is presented to demonstrate the capability of the constructed surrogate model, and for verification purpose the predicted results are compared with some of the *offline* analysis results that are not contained in the original data matrix used for POD.

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Thermodynamics-Informed Reinforcement Learning of Fluid Dynamics from Observation

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Key Words: Physics perception, Reinforcement learning, Fluid dynamics, Hybrid twins

In reinforcement learning (RL), an agent learns from the contact with the environment to perform a certain task. Such systems generalize experiences so that previously acquired knowledge is employed in new, but similar, goals. Model-based reinforcement learning helps to predict the output of actions based on simulations. In this scenario, the bottleneck of the approach is the model's accuracy to match reality. The correction of the model can be part of the RL optimization to learn an appropriate replica of the world.

We introduce a RL approach to correct fluid dynamics from the interaction with reality. We propose as a source model a data-driven physically informed digital twin of a glass full of a liquid based on the GENERIC formalism [1][2] to ensure the thermodynamical consistency of the simulation. The integration is performed in realtime from the solely evaluation of the free surface of the liquid, detected by computer vision techniques. From its study with recurrent neural networks we unveil the not measured information of the dynamics to perform the simulation.

The digital twin becomes a hybrid twin that learns to correct the deviations in the free surface reconstruction to maximize the similarity with the ground truth. The error is backpropagated through only a few activated layers of the whole architecture to preserve the patterns and useful insights already learnt from full field information. As a result, the reduced order space and the simulator are both adapted to the new, computational and real, liquids perceived.

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A Bending Consistent Meshfree Formulation for Reissner-Mindlin Plates

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The Reissner-Mindlin plate theory is attractive as it considers shear deformations through the thickness of a plate that can be applied to a broad range of engineering structures. However, it also suffers from the notorious "shear locking" when the plate thickness approaches the Kirchhoff limit. In the meshfree method, the employment of the nodal smoothing technique, as well as the higher-order reproducing kernel (RK) approximation, can easily satisfy the bending exactness (BE) and Kirchhoff mode reproducing condition (KMRC), which leads to a locking free meshfree solution [1]. Nevertheless, it is computationally inefficient due to the introduction of the smoothing cells and the larger kernel support size. To address this issue, in this study, we present a bending consistent Galerkin formulation that aims to fulfill the BE and KMRC efficiently. We first utilize the idea in the variationally consistent integration (VCI) [2] to correct the test function such that the residual of BE is automatically minimized. In this way, the smoothing procedure is bypassed, which speeds up the simulation. Then, to enable the use of a smaller support size, we introduce the quasi-consistent approximation technique in [3] with proper error control to avoid the moment matrix singularity in the RK approximation when a quadratic basis is used with smaller support size. In this way, the RK approximation still meets the KMRC, but the approximation construction is more efficient. For the stabilization of low energy instability in the proposed nodal integration framework, a variational multiscale stabilized (VMS) method [4] is used to eliminate the spurious oscillatory modes. The proposed framework is validated by solving various numerical examples, and the numerical results are locking-free and are more efficient than the conventional approaches.

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A Coupled Meshfree and Infinite Element Approach for Non-Fourier Heat Conduction Problems

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Key Words: *meshfree methods, infinite element methods, non-Fourier heat conduction, infinite domain, naturally stabilized, variational consistency conditions*

In this research, a stable and efficient meshfree/infinite element approach is introduced for solving a half-space with a heat source. The non-Fourier heat equation is used to obtain the finite thermal propagation speed. The unbounded properties of the semi-infinite domain defined as the far-field are simulated by infinite elements [1, 2]. Utilizing the infinite elements can reduce the size of the numerical model to save computing time. For the near field, a nodally-integrated reproducing kernel particle method (RKPM) is used. Meshfree methods are friendly for avoiding mesh issues such as mesh entanglement and mesh distortion. The nodally integration method is used in this research, and this method usually provides poor accuracy and unstable results in meshfree methods. These issues have been addressed using the naturally stabilized nodal integration [3] and variational consistency conditions [4]. The responses without a self-oscillation frequency are investigated. In addition, corresponding analytical solutions have been derived in the frequency domain. Finally, some conclusions are made and discussed by comparing the results obtained with the corresponding analytical solutions.

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A Stabilized Galerkin Mixed Formulation for Nearly Incompressible Material

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Key Words: *Mixed Formulation, Stabilized One-Point Integration, Strain Smoothing, Variational Multiscale Method*

The conventional numerical methods in modeling nearly incompressible materials usually suffer from "volumetric locking." Although the usage of the mixed formulation can alleviate the locking issue, the pressure oscillation occurs due to the violation of the LBB condition. Besides, low energy instability exists in conventional nodal integration methods in meshfree and mesh-based methods, such as SCNI [1] and SFEM [2]. This research develops a stabilized Galerkin mixed formulation within a one-point integrated framework for modeling nearly incompressible materials that bypass the abovementioned issues. The variational multiscale (VMS) formulation [3] is introduced to circumvent the low energy modes and LBB instability in the conventional Galerkin formulation. The multiscale decomposition of the variational equation results in a residual-based stabilized Galerkin framework. The derived fine-scaled terms act as a stabilization that mitigates the hourglass instability and pressure oscillation. The strain smoothing and strain divergence smoothing method is employed to ensure the satisfaction of the integration constraint in the new Galerkin formulation. A series of numerical examples under the incompressible limit are examined to verify the effectiveness of the new formulation. In numerical testing, the proposed method outperforms other conventional stabilization approaches [4].

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Iso-geometric Analysis Method for Thermal Fatigue of Wafer Level Chip Scale Package

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Key Words: *Solder Ball, Iso-geometric Analysis, Optimization, Constitutive Model, Thermal Fatigue, Fatigue Model*

The failure of electronic packaging often starts from the failure of solder. Solder balls are soldering materials used for chip-size ball-grid array package. The reason for the failure of the solder is that when the solder ball is subjected to thermal loading, the thermal stresses concentration occurs at the solder boundary due to the coefficient of thermal expansion (CTE) mismatches between different materials. This cyclic stress loading will produce irreversible deformations such as creep and plastic deformation. When the permanent deformation reaches a certain level, fatigue crack will propagate along the solder ball boundary and leads to failure. The current accuracy of evaluating the reliability of electronic packaging depends on the material constitutive model, finite element model and fatigue life prediction model. In this research, we use the optimized iso-geometric analysis (IGA) method for numerical simulation of thermal-mechanical coupled problem. The IGA method uses non-uniform rational B-splines (NURBS) as the shape function, which is a combination of B-spline and weight coefficients. In computer-aided design, due to the introduction of weights used to describe irrational functions, NURBS can accurately describe the geometry of solder balls. Compared with the finite element method, the IGA method can reconstruct the geometric field with fewer points. In the physical field, we introduce the optimization method, which treat both control values and weights as nodal variables. Therefore, we proposed an alternating iteration scheme, which uses the Galerkin weak form of governing equation to solve the control values, and then we update the weights by the least square method and Newton's method. The control values should also be updated for the new weight functions to obtain better physical solution. The constitutive equation used in this research is Anand model [1]. Anand model is mainly used to describe the nonlinear deformation behavior of solder balls. To calculate the Anand model, nine parameters must be determined and its stress and deformation resistance must be nonlinearly iterated [2]. Thermal fatigue refers to a progressive degradation of a material due to cyclic fluctuations in temperature. The fatigue model we chose is Coffin Manson's plastic strain-based model to predict low cycle fatigue, and Basquin's elastic strain-based model to predict high cycle fatigue. The results of this research found that the IGA method can reconstruct geometric and physical fields with fewer points than finite element method. Since there are fewer points, the calculation time can also be reduced.

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RBF WENO Reconstructions with Adaptive Order and Applications to Conservation Laws

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Key Words: *radial basis function; weighted essentially non-oscillatory; WENO-AO; RBF-WENO-AO; hyperbolic equation*

We develop a framework for finite volume radial basis function (RBF) approximation of a function u on a stencil of mesh cells in multiple dimensions. The theory of existence of the approximation is given. In one dimension, as the cell diameters tend to zero, numerical evidence is given to show that the RBF approximation converges to u to the same order as a polynomial approximation when the RBF is infinitely differentiable. Specific multiquadric RBFs on stencils of 2 and 3 mesh cells are proven to have this convergence property. A two-level RBF based weighted essentially non-oscillatory (WENO) reconstruction with adaptive order (RBF-WENO-AO) is developed. WENO-AO reconstructions use arbitrary linear weights, and so they can be developed easily for RBF approximations, even on nonuniform meshes in multiple dimensions. Following the classical polynomial based WENO, a smoothness indicator is defined for the reconstruction. For one dimension, the convergence theory is given regarding the cases when u is smooth and when u has a discontinuity. These reconstructions are applied to develop finite volume schemes for hyperbolic conservation laws on nonuniform meshes over multiple space dimensions. The focus is on reconstructions based on multiquadric RBFs that are third order when the solution is smooth and second order otherwise, i.e., RBF-WENO-AO(3,2). Numerical examples show that the scheme maintains proper accuracy and achieves the essentially non-oscillatory property when solving hyperbolic conservation laws.

Solving large-scale engineering problems by ghost point method and domain decomposition method

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Key Words: *meshless methods, ghost point method, domain decomposition method*

In this study, a meshless numerical model, based on ghost point method and domain decomposition method (DDM), is proposed to analyze large-scale engineering problems. The ghost point method is one of the newly-developed meshless methods, which can avoid the time-consuming tasks of mesh generation and numerical integration. The ghost points method adopted the concept of ghost points to improve the conventional Kansa's method by separating the collocation points and the source points and extending the source points to a covering domain region. As a result, this simple process of the ghost point method can significantly increase the stability and accuracy of the Kansa's method. In order to determine the optimal shape parameter of the radial basis function, the modified Franke's formula and the leave-one-out cross-validation (LOOCV) algorithm are adopted in this study. However, the full-populated system of linear algebraic equations in the ghost point method limits the applicability to solve large-scale engineering problems. In this study, the ghost point method cooperates with the DDM to reduce the requirements of huge computers resource when the large-scale engineering problems are considered. Several numerical examples will be provided to verify the feasibility, accuracy, and stability of the ghost point method combined with the DDM to solve large-scale engineering problems.

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A class of Laplacian and mixed derivative models in the SPH framework

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Key Words: 2nd order consistency, Laplacian, Mixed derivative

Smoothed Particle Hydrodynamics(SPH) and Moving Particle Simulation(MPS), which are both mesh-free particle method with the Lagrangian description, have high potential for simulating free-surface flows. Both SPH and MPS have weakly incompressible and incompressible schemes, but weaknesses may remain especially in the second-order differential model with Laplacian operator and mixed derivatives. Although the gradient operator in SPH uses a renormalization to overcome the weakness in the case of non-uniform particle distribution, the conventional Laplacian operator in both SPH and MPS loses accuracy in the case of non-uniform particle distribution.

Recently, the Least-Square MPS(LSMPS) [1] gives consistent higher-order differential operators, and the convergence profiles of these operators show good results not only for uniform particle distributions, but also for non-uniform particle distributions. A similar corrections for Laplacian and mixed derivative operators in SPH have been proposed by Fatehi and Manzari [2] and Lian et. al. [3], but there is no clear discussion of their similarities and differences.

In this study, we reformulate the second-order derivative operator including the Laplacian and the mixed derivative using the consistency of the Taylor expansion in order to preserve the predicted truncation error. The convergence of the Laplacian and mixed operators is verified for several influence radii of SPH, and the relationship between the existing and proposed models is shown.

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A coupled 3D isogeometric/least-square MPS approach for modeling fluid–structure interactions

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Key Words: *Isogeometric analysis; MPS method; Coupling algorithm; Fluid–structure interaction*

A two-way coupling method of the three-dimensional (3D) isogeometric approach and the least-square moving particle semi-implicit method (LSMPS) is presented for handling the fluid–structure interaction problems. This method takes advantages of isogeometric analysis (IGA) for structure deformation, e.g. the exact representation of the structure geometry and high accuracy for solution fields with relatively few elements, and that of the LSMPS method for fluid flow, e.g. its consistent discretization for both internal particles and boundary conditions. When the fluid is solved by the LSMPS method, the NURBS (Non-Uniform Rational B-Splines) surfaces provide boundary conditions for the LSMPS method. Afterward, the pressure on the NURBS surface is first evaluated from the pressure and the corresponding derivatives at the LSMPS particles by using the Taylor series expansion, and then integrated to determine the pressure force at the virtual points on the NURBS surface by using the Newton–Cotes method. Subsequently, the pressure forces at the virtual points are distributed onto the control nodes (i.e. control points) of the IGA elements so that the structure deformation can be analyzed by using the IGA method. The coupling algorithm is based on a Lagrangian framework and can handle the boundary conditions and the fluid–structure interactions accurately and easily. Finally, three examples, i.e. fluid flowing in a rigid pipe, fluid-tank, and fluid-torus interactions in the elastic regime, are simulated to demonstrate the accuracy and validity of the proposed coupling method.

Acknowledgment

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A Multiphase Axisymmetric Model of Moving Particle Semi-implicit Method

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The moving particle semi-implicit method (MPS) is a mesh-free particle method, which has great advantages in dealing with large deformation problems due to the Lagrangian nature. However, for the MPS method, the neighbor particle list is updated in each time step, thereby resulting in extensive calculation. Given the significant increase of particle number for the 3D simulation, the high computational cost of the original MPS method limits its application in handling the 3D axisymmetric problem. To improve the computation efficiency of the particle model, scholars have explored the axisymmetric model suitable for the smoothed particle hydrodynamics (SPH) method. These axisymmetric SPH models [1] have been proved to have the ability to significantly reduce the calculation cost. Nevertheless, an axisymmetric model applicable to the MPS method has not been published in the literature.

In this study, a multiphase axisymmetric-MPS model based on the Cartesian coordinate system was developed to deal with 3D axisymmetric problems. In the proposed model, as shown in Fig. 1, the virtual rotating particles are applied to supplement the neighbor particles of the particles of the 2D plane for considering the hoop stress and the Langrangian interpolation characteristics. The divergence, gradient, Laplace operator, and PPE models are re-established to consider the interaction among virtual rotating particles and rotating surface particles. To test the accuracy and stability of the model, the case of the cylindrical capillary jet breakup [2] is simulated.

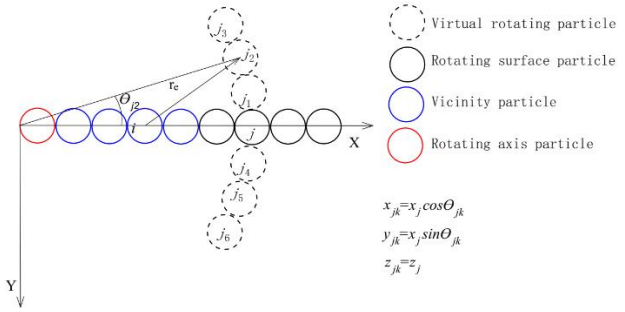

Fig. 1. The initial particle distribution of the axisymmetric-MPS model

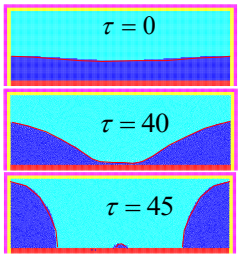

Fig.2. Comparison of the present instantaneous interface with reference results[2] (red line)

The initial configuration of the long cylindrical capillary jet details in Ref. [2]. At the density ratio $\rho_2 / \rho_1 = 0.8$, the disturbance wave number $k = 0.7$, viscosity ratio $\mu_2 / \mu_1 = 0.01$, and Reynolds number $Re = 1$, Fig. 2 shows the instantaneous interface of the capillary jet in the 2D rotating axial section simulated by the method proposed herein. The good agreement shown in Fig. 2 indicate that the perfect reproduction of the procedure of the capillary jet breakup tests the accuracy and stability of the model.

Key Words: *Particle method, Axisymmetric-MPS, Multiphase, Virtual rotating particles*

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A Particle Method for Strongly Coupled Simulation of Incompressible Fluid and Rigid Bodies with Velocity-Based Constraints

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Key Words: *Particle Method, Linear Complementarity Problem, Incompressible Fluid, Rigid bodies*

In this study, we propose a method to achieve strongly coupled calculations of incompressible fluids and rigid bodies using the particle method. The proposed method is based on the authors' previous study [1] and adopts a velocity-based formulation and derives a linear complementarity problem as an equation to obtain the pressure due to the requirement that no attractive force is generated between particles. This linear complementarity problem is also used for contact between rigid bodies, and by solving the constraint conditions for incompressibility and contact between rigid bodies, as well as the constraint conditions for the interaction between rigid bodies and incompressible fluid in the same way, strong coupling between incompressible fluid and rigid bodies is accomplished.

Furthermore, we introduce velocity-based constraint conditions that generalize the nature of the constraint conditions required to perform the strong coupling calculation using the same method, and propose a more flexible and versatile system for the strong coupling calculation that can be applied to other than incompressible fluids and rigid bodies.

In order to validate the method, we show examples of calculations performed to confirm that the method correctly calculates the behavior of a rigid body, the behavior of an incompressible fluid, the interaction between a rigid body and an incompressible fluid, and the strong coupling. The examples include calculations for scenes consisting only of rigid bodies, hydrostatic pressure calculations, calculations for dam break problems, and calculations for buoyancy forces, etc.

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31 July–5 August 2022, Yokohama, Japan

Addition/Deletion-based Multiresolution LSMPS with Multi-time-stepping

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Key Words: Particle method, Multi-resolution, Particle addition/deletion, Error estimation

Particle methods are well-suited to model complex fluid phenomena such as multiphase and free-surface flow. In recent years, several successful multi-resolution particle implementations have been proposed based on prescribed high- and low-resolution sub-domains. However, speed-ups are limited for many applications, such as for multiphase and free-surface flows, where the high-resolution regions are moving in time.

In this study, an adaptive multi-resolution scheme is considered based on error estimation. Specifically, the error estimation is defined by the local truncation error for the LSMPS spatial discretization of velocity. In [1], particles were resized based on the error estimation. This technique gave accurate and stable results for a two-dimensional rotating cylinder problem with a small clearance. However, the application is limited to when the critical regions changes slowly in time. To increase applicability, particle addition and removal schemes have been incorporated to handle faster resolution changes. To reduce pressure fluctuations, particle addition and removal occur over several time-steps by using a time-dependent weight function. Its performance has been evaluated for Karman vortices.

Time-marching schemes for particle methods are seldom fully implicit. Therefore, the time-step length is typically restricted by the smallest particle sizes. To handle this issue, time-step length restrictions are applied to the fluid particles individually. This enables the use of longer time-step lengths for most particles. The main challenge with the multi-time-stepping is the implicit pressure calculation at intermediate time-steps when not all particles are updated. In this study, the pressure is either assumed to be constant during a time-step or that only the low-frequency part of the pressure field changes. The latter option can be implemented by using a multigrid solver with high-frequent smoothing only over updated particles.

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Analysis on molten material spreading behavior with Moving Particle Hydrodynamics method

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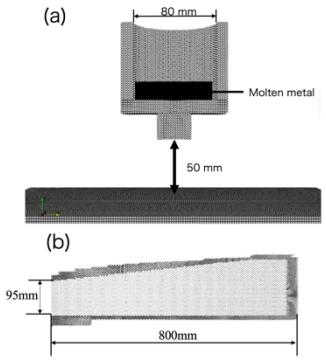
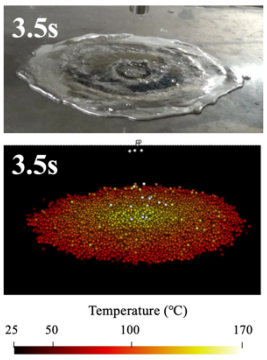
Key Words: *Particle method, Melt spreading, Nuclear Severe Accident, Solidification,*

During a postulated nuclear severe accident, molten material called corium spread on the containment floor at Primary Containment Vessel (PCV). Moving Particle Hydrodynamics method (MPH method) [1,2] which is a new particle method has advantages to simulate the melting and solidification, where the solid and the liquid coexist. In this paper, the corium spreading behaviours were analyzed with the MPH method.

The 2 different experiments were analyzed with the MPH method. The calculation geometry was summarized in Fig.1. In Fig.1 (a), the low-viscosity molten metal discharged from the vessel and spread on the stainless plate with a flat surface. In Fig.1 (b), the high-viscosity molten material spread on a ceramics plate.

The simulation result using the low-viscosity material was shown in Fig.2. The molten metal drastically spread in short time with a flat surface and the solidification started from the edge of the metal. The molten metal solidified in circle shape. Fig.3 is the results of the highly viscous spreading behavior [3]. Unlike Fig.2, the molten corium spread gradually on the ceramics substrate and solidified due to the radiation from the free surface. The results indicated that the MPH method was capable of simulating the corium spreading behavior in the nuclear severe accidents.





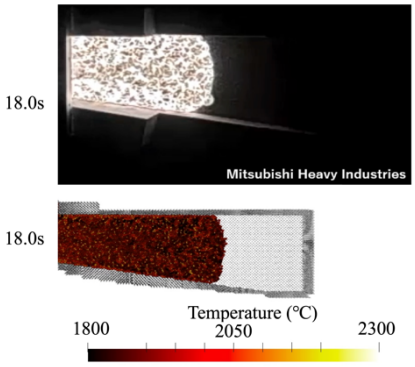


Fig. 1 Calculation geometry Fig. 2 Melt spreading with low-viscosity Fig. 3 Corium spreading with high-viscosity

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Application of Moving Particle Hydrodynamics Method to Fluid Lubrication Problems in Line Contact

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Key Words: *Particle methods, MPS, MPH, SPH, CFD, Fluid Lubrication*

Nowadays, energy and resource saving is significantly required in order to realize a sustainable society. In that context, fluid film lubrication of machine elements such as bearings, which leads to smooth movement by avoiding metal-to-metal contact and wear, is essential to operate a mechanical system in well-functioning conditions. As for the fluid film lubrication, lowering friction loss and extending bearing life are strongly demanded for the sake of energy and resource saving. The straightforward approach is to achieve the fluid film lubrication with small amount of lubricant to reduce stirring and sliding friction losses in bearings. Therefore, it is important to understand and predict the detail of lubricant behaviour and distribution in an entire bearing. And the computational fluid dynamic (CFD) is expected to be a promising approach to realize that.

Considering practical machine elements such as bearings, a meshless, Lagrangian, particle-based method is considered to be a promising approach since it is more suitable to model free surfaces, moving or deforming boundaries, multi-phase flows, and complex geometry than the conventional grid methods such as the finite volume method. In this study, a physically consistent particle method, the moving particle hydrodynamics (MPH) method,[1] was applied to the fundamental fluid lubrication problems: the wedge film and the squeeze film in order to confirm its capability. The compressible version of the MPH method, so-called MPH-WC,[2] was employed here. The computed pressure profiles induced in the wedge and squeeze films were validated against analytical solutions based on the classical Reynolds equations[3] and good agreements were confirmed.

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Development of an Interface Tension Model of MPS Method to Avoid Particle Clumping of Inner-Particles

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Key Words: *MPS method, Multiphase flow, Interface Tension, Potential Model*

Background and Objective

For capturing the complicated dynamics of surface, Moving Particle Semi-implicit (MPS) method has been increasingly utilized in diverse fluid problems. As one of the major types of methods to model surface tension, potential model [1][2] has been widely applied to the relatively complex surface dynamics thanks to its simplicity and stability. Recently, a new potential model to consider the "interface tension" between fluid-fluid interface as well as ordinary surface tension has been developed [3]. However, in the preceding potential models, the potential force acts not only on the surface/interface particles, but also on the particles inside the fluid bulk, leading to "particle clumping" involving the unrealistic hindering of fluid flow. Moreover, the preceding potential models require surface tension coefficients of fluids even when only fluid-fluid interface is considered, and no surface exists [3].

In this study, a new potential model has been developed for the fluid problem involving only interfaces, and no surface. With this model, potential force acts only on the particles on the vicinity of interfaces, avoiding the particle clumping and unnecessary requirement of surface tension coefficients of each fluid.

Developed Method and Validation

Based on the methodology proposed by Kondo et, al. [2], a new interface tension model with a new concept of "interface potential" has been introduced. The interface potential is defined only effective when particle i and its neighbor particle j belong to different fluid phases and is calculated with a coefficient determined only by the interface tension coefficient between these two phases. In this way, the potential force, which is derived as the negative of spatial derivative of interface potential, acts only on the particles on the vicinity of the interface of different phases.

The current model has been validated against the Taylor's shear flow problem and the result has been compared with the Zhu's existing interface potential model [3]. Since Zhu's model require surface tension coefficients of each fluid, which theoretically does not influence the prediction of Taylor's shear flow problem, they were determined arbitrary. However, in Zhu's model, the particles of the fluid bulk clumped due to the attractive force calculated by arbitrarily determined surface tension coefficients, leading to the failure to correctly model the influence of interface tension. On the other hand, the current model, which is based only on the interface tension coefficient, does not involve such particle clumping and the result relatively agreed with theoretical value.

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Development of elastic structure model and fluid-solid coupled model in MPS method

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Abstract: Based on the moving particle semi-implicit method (MPS), an elastic structure model and coupled solvers for fluid structure interaction is developed. The elastic structure model adopts Lagrangian kernel function and is discretized in Lagrangian system to ensure that the simulation process is more in line with the physical reality and avoid tensile instability. And Euler kernel function is used in fluid calculation. The fluid-solid coupled process is realized by sharing the load, velocity and position information of the solid boundary. The developed models are verified by the free oscillation of cantilever beam, violent sloshing test and dam break with elastic gate.

Development of Parallel Parametric Analysis System Using Coupling-Matrix-Free Iterative S-version FEM for Design of Structure with a Hole

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Key Words: *Parametric Study, S-version FEM, Parallel Computing, Message Passing Interface*

Operators of the V-bending process have sometimes been injured because of broken pieces of a die. To prevent this accident, a structure of the die that is tough to break is required. In the previous study [1], we performed parametric studies of the V-bending die with a hole using the Coupling-Matrix-Free Iterative s-version FEM (CMFI s-FEM) [2]. In this method, because the mesh for the whole analysis domain and the mesh in the vicinity of the hole were created separately, it was not necessary to perform remeshing in a parametric study of the hole coordinates. However, there were two issues. The first one was computation time. Such parametric study needs several hundred thousand cases of analyses. Thus, the analyses took a very long computation time. The second issue was that it required a considerable amount of effort to perform the analyses manually.

In this study, to overcome these issues, we developed a parallel parametric analysis system. We implemented this system based on the Message Passing Interface (MPI), to perform a parametric study on a distributed-memory parallel computer such as supercomputers and PC clusters. In the parallel parametric analysis system, each analysis with a parameter such as the coordinates of a hole is assigned to an MPI process. Every analysis in the parametric study is computed completely in parallel.

A structure with a hole was analyzed for a demonstration of the parallel parametric analysis system. The shape of the hole was assumed to be an ellipse. As parameters of the parametric study, the central coordinates, the semi-major axis, the semi-minor axis and the angle of the elliptical hole were used. We evaluated the parallel performance, the computation time, and the convergence performance of the iterative solver of the parallel parametric analysis system based on CMFI s-FEM.

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Development of snow accretion analysis method for railway vehicles

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Key Words: *Snow accretion analysis, Airflow analysis, Coupled analysis, Railway vehicles*

In case where a train travels on the snow covered tracks, snow accretes to train bogies and grows up. When the accreted snow drops off the train bogies, it might damage the railway ground facilities along the tracks, the train devices, etc. To establish countermeasures against such snow accretion damage, we have developed a snow accretion analysis method in order to understand the snow accretion process.

The “snow accretion analysis method” developed by this research consists of an “airflow calculation”, a “trajectory calculation” and a “snow accretion calculation”. In the snow accretion analysis method, airflow velocity is obtained by the airflow calculation, trajectory of flying snow particles is calculated by the equation of motion for gravity and drag using the airflow velocity, snow accretion determination for objects is performed by the snow accretion calculation. When a certain amount of snow accretes to the objects, the accretion shape was suitably taken into consideration in the airflow calculation. We calculate again the airflow velocity using the updated accretion shape and the snow accretion growth using the updated airflow velocity.

In the snow accretion calculation, the theoretical principle is not yet established in the snow accretion phenomenon, and there are many unexplained parts. Therefore, in this research, we are developing the snow accretion determination algorithm by the experimental method. It has been confirmed by the snow accretion experiment that the snow accretion shape has a snow accretion angle according to the speed and property of the flying snow particles. In order to incorporate these experimental results, a snow accretion determination algorithm by the velocity and collision angle of the flying snow particles have been developed.

In this research, two kind of validations are performed using a snowfall wind tunnel. First, a snow accretion analysis on a cubic model is performed, and it was confirmed that the snow accretion analysis reproduces the snow accretion experiment with a relative error of 6%. Next, each snow accretion analyses on two railway car-body models are performed, and it was confirmed that the snow accretion distributions were similar with the experiments. As this result, it became possible to consider places and causes where snow accretion occurs for the railway car-body models by the snow accretion analysis.

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Extended B-spline-based implicit material point method enhanced by $\bar{\mathbf{F}}$ projection method

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Key Words: *Material point method, Extended B-spline basis function, F-bar projection, nearly incompressibility, Nitsche's method*

A novel computational method incorporating the F-bar projection method into extended B-spline-based implicit material point method (EBS-MPM) is proposed to avoid not only volumetric locking but also stress oscillations. MPM with the standard B-spline basis functions is capable of suppressing the cell-crossing error caused by particles crossing background grid boundaries and reducing the quadrature error. Furthermore, EBS-MPM enables us to avoid both stress oscillations arising from inaccurate numerical integration and ill-conditioning of their resulting tangent stiffness metrices thanks to extended B-splines (EBS) which are active on the background grid containing smaller number of material points than interior ones. In addition, boundary conditions are imposed arbitrarily by the application of the Nitsche's method, while the capability of conventional MPMs is limited [1]. Although the applicability of EBS-MPM to nearly incompressible and plastically incompressible material problems was investigated, it has been confirmed that volumetric locking was avoided by higher-order EBS, but stress oscillation was not [2]. Various countermeasures against incompressibility have been proposed, but incompressible constraints are interpolated by basis functions lower than those for displacement in most of them. Since higher-order EBS are preferably utilized to suppress the cell-crossing error in EBS-MPM, it is necessary to reduce the order of basis functions appropriately. Therefore, we incorporate the $\bar{\mathbf{F}}$ projection method into EBS-MPM in this study, which showed the efficacy to solve nearly incompressible problems with a pure displacement formulation using higher-order basis functions [3]. This is expected to be a novel stabilizing scheme for MPM which is able to avoid volumetric locking as well as stress oscillations due to incompressibility. In the presentation, several representative numerical examples are presented to demonstrate the performance of the proposed method.

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Impulse-Based DEM for Boosting Simulations of Particulate Materials

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Key Words: Discrete Element Method, Granular, Event-Driven, Impulse-Based Simulation

The Discrete Element Method (DEM) models collision of particles as a spring-dashpot system[1]. The eigen frequency obtained from the oscillation equation defines an upper limit of the time steps in DEM. Since higher stiffness of the spring for accurately modeling the collision requires smaller time step, DEM-based computations tend to require high computational cost. In other hand, the event-driven algorithm, which adopts an impulse-based expression of the collision and solves all binary collisions by analytically determining the trajectory of particle motions, is developed in studies on molecular dynamics[2]. It represents the time evolution by varying time steps according to the collision events, and there is no upper limit of the time steps for stability of computation such as DEM. However, the time steps become zero when the collision frequency is very high. In addition, this algorithm has the inherent sequential nature which prevents parallelization unless special implementation.

In this study, we propose Impulse-Based DEM (IB DEM). We locally applies the event-driven algorithm to achieve stable and accurate simulation with relatively large time steps. Our proposed method determines the motion of each particle based on known values of its neighboring particles in the previous time step, which are inside the local region centered on the particle. The event-driven algorithm is applied to the calculation in the local region assuming that velocities of particles are constant in the time step. Moreover, our proposed method can be parallelized because each particle is calculated independently. We show results of analyzing bead mills by IB DEM.

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Large-deformation analysis of saturated soils using extended B-spline-based implicit material point method

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Key Words: *Material point method, Saturated soil, Extended B-splines*

Extended B-spline-based implicit material point method [1] is developed for the coupling analysis of a saturated soil with the aim to simulate a collapse process of ground structure, which is mainly caused by seepage flow in a long time scale and involves transition processes from a solid to flowing mixture. The governing equations are formulated based on the full formulation [2] of the theory of porous media, in which primary variables are solid displacement, fluid velocity, and fluid pressure. This formulation realizes the simulation of pore fluid flow in a highly permeable porous structure as shown after collapsing the structure skeleton. The continuum body of the solid skeleton is discretized with a set of Lagrangian material points that possess the information of the solid and liquid. In order to improve the robustness and efficiency in comparison with the previous studies, we apply an implicit scheme enhanced by extended B-splines (EBS) [3]. At the same time, with the aim to weakly impose an arbitrary boundary condition of saturated soil, such as permeable/impermeable surface, Nitsche's method is introduced with boundary points. Also, the stabilized method based on the variational multiscale method is utilized for the stabilization of the pressure fields without losing continuity characteristics of B-spline basis functions. Several numerical examples are simulated to demonstrate the performance and capability of the proposed method in stably solving the large deformation of solid skeleton and flow of pore fluid.

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Modelling of Interface Tension using Multi-resolution MPS Method with Polygon Boundary

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Key Words: *MPS (moving particle semi-implicit) method, Polygon wall, Multi-resolution, Surface tension*

Simulation of severe accident in nuclear reactor involves multiphase flow phenomena with free surface or component interfaces. The moving particle semi-implicit (MPS) method [1] waives the topological mesh which has been extensively employed in multiphase simulation. In the traditional MPS method, the uniform-size particles are utilized, which leads to high computation cost when high spatial resolution is demanded in the region of interest, e.g., near the phase interfaces [2]. Meanwhile, a large number of wall particles are employed to model the wall boundaries, which further increases the computation resource.

In order to improve the computation efficiency and accuracy, the multi-resolution method [3] and polygon boundary [4] are implemented into the MPS method. In order to accommodate with the non-uniform particle size, several basic models of the MPS method are modified, including particle effective radius, gradient operator model, Laplace operator model, and free surface identification model. Based on dam-break simulation, it is verified that utilization of multi-resolution particles can capture more complex free surfaces. The polygon boundary eliminates the wall particles. The wall distance and background grid are introduced to calculate the contribution of the boundary to fluid particles. The zero-pressure gradient at the wall is realized with the virtual mirror particles about the wall. For the verification of the polygon algorithm, the static pressure in a water column is simulated. The discrepancy between the pressure at the monitoring point and the theoretical value is 6.25%.

In this paper, potential force interface tension model [5] is improved to expand its application to multi-resolution particles. Four sets of coefficients are calculated when the particles are in two sizes, namely large-large, large-small, small-large, and small-small coefficient. After selecting the corresponding coefficient, the potential force can be calculated between fluid particles. Regarding the wall contact cases, temporary wall particles are set in the range of the effective radius of the particle. To verify the accuracy of the contact angle, a floating droplet is simulated which shows accurate prediction between fluids. In addition, the wall contact angle is simulated and the predicted value agrees well with the theoretical one. Therefore, the improved interface tension model can be applied to the multi-resolution simulation.

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Moving Particle Semi-implicit/Simulation Method with Bottom Boundary-Fitted Coordinate Transformation

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Key Words: *Mesh-Free Particle Method, MPS Method, Boundary-Fitted Coordinate Transformation*

We propose an effective numerical method for simulating ocean waves based on a mesh-free particle method with a bottom boundary-fitted coordinate transformation. While particle methods such as the smoothed particle hydrodynamics (SPH) and the moving particle semi-implicit/simulation (MPS) method have been applied to simulations of free-surface flows including tsunamis [1, 2], they have difficulty in handling curved boundary such as seabed. Though an existing study has proposed the curvilinear SPH [3], which adopts a coordinate transformation corresponding to bottom boundaries, the curvilinear SPH has mainly focused on simulation of inviscid flow ignoring the viscous term.

This study proposes a bottom boundary-fitted coordinate transformation for the Navier–Stokes equations considering the viscous term. We adopt the explicit MPS method as a mesh-free particle method, where pressure field is explicitly computed instead of solving the pressure Poisson equation. We derive a mixed derivative model of the MPS method since the coordinate transformation of viscous term generates the mixed partial derivatives. Our proposed method including the derivative model is verified by the simulation of a hydrostatic pressure problem with round-shaped bottom.

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Moving Surface Mesh-incorporated Particle Method Applied to Viscoelastic Fluids

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Key Words: *Particle method, Viscoelastic fluid, Weissenberg effect, Oldroyd-B model*

The polymer industry is interested in free-surface flow of viscoelastic fluids. Normal stress differences cause unique behaviors known as Weissenberg effect and so on. In this study, a new particle method was developed to predict the behavior, free-surface flow under normal stress differences. Up to the present, a number of numerical methods haves been developed for free-surface flows. In this study, the moving surface mesh-incorporated particle method developed by Matsunaga *et al*. [1] was used. In this method, the free-surface boundary can be more rigorously treated by using a surface mesh. The LSMPS scheme [2] was used as the spatial discretization method. Oldroyd-B model [3] was adopted as a viscoelastic model, with which an analytical solution can be derived for the test case considered in this study.

To examine the accuracy of the proposed method, problems where the Weissenberg effect occurs were simulated. The Weissenberg effect, also known as rod-climbing effect, is a typical phenomenon of viscoelastic fluids. Surface shape computed by proposed method with coarse spatial resolution didn't match the curve calculated by a finite element method in the previous study [4]. On the other hand, the shape computed with fine spatial resolution was close to the curve of previous study. Thus, it is implied that the result obtained by using the proposed method with the fine resolution has a comaparable accuracy to the previous study. To compare climbing heights between numerical results and theoretical solution [5], numerical simulations were performed at several Weissenberg numbers. Numerical results were in good agreement with theoretical solutions in lower Weissenberg numbers. Reproducibility of theoretical solution reduced as the Weissenberg number increases. However, it was confirmed that the results with fine resolution is close to theoretical solution. Through several basic problems, the proposed method is found to have the capability to reproduce Weissenberg effect. Hence, it is expected that the proposed method is able to predict other behaviors of free-surface flow caused by normal stress differences.

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MPS-WCMPS coupled method for bubble dynamic with density and pressure discontinuity

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Key Words: *MPS method, Weakly-compressible MPS, Bubble rising, Pressure discontinuity, Large density ratio*

Bubble dynamics are common encountered in a wide range of engineering applications. However, abrupt density and pressure drop would occur at the interface due to the discontinuity of fluid properties, e.g., density, viscosity and surface tension. Owing to the mathematical discontinuity, numerical simulation of bubble dynamics, especially for large density ratio, is always challenging.

The Lagrangian particle methods, such as the Moving Particle Semi-implicit method (MPS) [1], have attracted great attentions in simulating free surface and multiphase flows due to its distinct advantage in tracking moving interfaces.

This study presents a new coupled particle method for bubble dynamic with large density ratio. The proposed scheme couples the incompressible MPS and Weakly Compressible MPS [2], representing the liquid and gas phases, respectively. The liquid-gas phase interface is explicitly represented by a moving interface mesh, consisting of discrete nodes. The stress balance equations at the interface are adequately enforced on these interface nodes. The surface tension is considered as pressure jump at the interface [3] rather than treated as volume force. Without applying the smoothing or averaging scheme, the density and viscosity are preserved discontinuous across the interface. Benefiting from the least squares scheme [4], axisymmetric formulation is straightforwardly introduced. To save computational cost, a multi-time step algorithm is developed further. Moreover, to maintain quasi-irregular particle distribution and control the multi-spatial resolution dynamically, a user-defined particle shifting scheme is proposed.

Several benchmark tests are conducted to verify the accuracy and efficiency of the developed method. Satisfying agreements are obtained by comparing with reported numerical solutions and experimental data.

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Multiple solvers for implicit temperature calculation of plate heat conduction with MPS method

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In this study, an implicit algorithm and different solvers for temperature calculation were used to reduce the computation time of a plate heat conduction. The method used is based on the Moving Particle Semi-Implicit(MPS) method. The original MPS method uses explicit method for temperature calculation and is limited by time increment due to diffusion number especially in some cases with high thermal diffusivity. In this paper, the heat conduction of plate with Dirichlet boundary condition and Neumann boundary condition are studied. Furthermore, we contrast with steady state and transient heat conduction. The calculation time and accuracy of explicit and implicit calculation of plate heat transfer cases are compared. In addition, different algorithms and existing solvers are used to calculate the implicit temperature equation, and the calculation time and accuracy of different algorithms and solvers are compared. Consequently, it is shown that the temperature obtained using implicit algorithm agrees well with that obtained using the original explicit algorithm and the steady state equation, the computation time of implicit algorithm is shorter than that of explicit algorithm. In addition, the coefficient matrix of implicit temperature calculation equation is similar to the Pressure Poisson Equation(PPE), the optimal solver can also be extended to the solution of PPE.

New Spar Type Floating Wind Power Plant Behavior Simulation by SPH Method

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Key Words: *Particle Method, Smoothed Particle Hydrodynamics, Wind Power Plant.*

It is important to stabilize behaviors for the efficiency of the floating wind power plants. And it is necessary to consider safety in the case of a design for the floating wind power plant about the natural disasters such as tsunamis. To predict behaviors of floating wind power plants in the ocean are very important for the safety and the ability of efficiency for power generation by numerical simulations. The particle methods which are the smoothed particle hydrodynamics (SPH) method [1] and the moving particle semi-implicit (MPS) [2] method are recently applied to fluid dynamics analyses for predictions for behaviors of structures under natural disasters such as Tsunami.

The SPH method including the artificial viscosity coefficient and the artificial density diffusion coefficient are proposed by M.Antuono et al.[3] and D.Molteni et al.[4] that is the δ-SPH method. The numerical correction terms are added to the momentum conservation equation and mass conservation equation in the δ-SPH method respectively. The 3-dimensional δ-SPH method analyses are applied to calculate the behaviour of new spar type wind power plant models. The calculated results are compared with the experimental results of the new models of the experiments.

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Numerical Analysis of Wave Pressure Acting on a Ship by a Multi-Resolution Particle Method

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Key Words: *MPS, SPH, Ship-wave Interaction, Wave Force, Computational Cost*

We developed a numerical analysis method that can predict the wave pressure acting on a ship in a short computation time [1]. The method is based on the overlapping particle technique for the multi-resolution simulation of particle methods [2] and ellipsoidal particles [3]. The spatial resolution can be changed in three levels in the simulation domain. The spatial resolutions of this simulation can be set more flexibly than conventional single- and two-level spatial resolutions. In addition, OpenMP, which is a parallelization library, was used to parallelize the simulation program.

Using the developed method, the wave pressure acting on the ship bow under short regular waves was numerically analyzed. The results revealed that the wave pressure values obtained by the numerical simulation was close to the experimental values. The total number of required particles was reduced by approximately 99%, compared to the case where the multi-resolution method was not applied. Future issue is simulation under long waves, where ship motion should be considered.

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Numerical investigation of Particle Deposition on Substrates in Cold Spraying by SPH Method

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Key Words: *SPH Method, Cold Spraying, Deposition, Interfacial Force Model*

Due to the characteristics of high velocity, high pressure and small size, it is difficult to observe the particle deposition process of cold spraying in the experiment, so the numerical simulation called virtual experiment becomes more important tool. In this paper, smoothed particle hydrodynamics method is used to simulate the particle deposition process of cold spraying. Based on SPH theory, related numerical techniques and conservation equation of continuum mechanics, a dynamic impact model of cold sprayed particles impinging on substrate is established. With the help of the L-J atomic potential model, a new interfacial force was proposed, which can be successfully used to predicted the critical velocity of particle deposition according to the increase of surface temperature, to eliminate the rebound of the deposition particles. The effects of several particle shapes and subsequent impact position are also discussed. Result shows that, compared with elliptic particles, circular particles are more conducive to deposition, and different positions of subsequent particle impact have significant effects on coating quality. In this paper, the model of cold spray particles impinging on the substrate established by SPH method can well reproduce the experimental phenomenon, which is helpful to understand the mechanism of particle deposition.

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On the bound solution property of the Node-based Smoothed Point Interpolation Methods (NSPIMs) in coupled problems of porous media

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Key Words: *Coupled analysis, Saturated porous media, poro-elasticity, Node-based smoothed point interpolation method, upper bound*

An outstanding feature of the node-based smoothed point interpolation methods (NSPIMs) in solid mechanics problems is their potential to yield softer stiffness matrices compared to those of the linear finite element method (FEM). In particular, it has been shown that the NSPIM with linear shape functions yields the upper bound of the exact solution in energy norm in elasticity problems in contrast to the lower bound property of the solutions obtained using the linear FEM. Accordingly, the solution of the NSPIM with linear shape functions together with the solution of the linear FEM can bound the exact solution in solid mechanics problems. In this study, bound properties of the NSPIMs and linear FEM are examined in plane-strain coupled problems of porous media, to explore how the presence of pore water pressure affects this feature of the NSPIMs and linear FEM. The bound properties of the solution of three popular NSPIMs and linear FEM in poro-elasticity problems are then thoroughly investigated. The results show that the upper bound solution property of the NSPIMs is lost in coupled problems of poro-elasticity due to the coupling effects of the fluid phase.

Particle Method Simulation of the Eutectic Liquid Formation in Sn-Bi system using PHALSER Code

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Key Words: *Particle method, Simulation, Eutectic liquid, PHALSER*

Particle method is suitable for the simulation of melting, relocation and solidification of materials in a severe accident analysis of nuclear power plant and it has been applied for simulating various phenomena such as the candling of fuel rods, melt spreading of corium, molten-corium-concrete interaction (MCCI), and so forth. In those severe accident phenomena, liquid phase is formed even below the melting temperature of the material by eutectic reaction which occurs at the interface of different materials. In the boron-carbide control rods, for example, eutectic liquid is formed at the interface of the boron-carbide and SUS, which significantly affects the following accident scenario [1]. Therefore, development of a model to predict the behavior of the eutectic liquid formation is important for severe accident simulation.

In the present study, a test was conducted to investigate the dynamic behavior of the eutectic liquid formation. In the eutectic melting test, a solid cylinder of tin was soaked in a eutectic liquid pool of Sn-Bi which was maintained at a constant temperature slightly above the eutectic temperature. The solid cylinder was rotated to form a flow field in the pool and the weight of the solid was recorded to evaluate the rate of the eutectic melting. The test was conducted with changing the size of the cylinder or the rotation speed. It was observed that the rate of the eutectic melting at the solid surface is significantly dependent on the surrounding flow conditions and it can be explained by a film mass diffusion theory [2] when the flow is in the Laminar range.

On the basis of these observations, a eutectic reaction model was developed and implemented in a particle method code PHALSER [3] to perform the numerical simulation of the eutectic melting test. In the simulation, the tin cylinder and Sn-Bi pool was modelled using solid particle and fluid particle, respectively. The mass concentration of tin and bismuth was given as variables to both types of particles and their concentration over time due to diffusion was evaluated. The mass transfer at the interface between solid tin and Sn-Bi liquid was defined to be proportional to a mass transfer coefficient k_m, which was measured by the eutectic melting test. The solid tin particle was transformed to the Sn-Bi liquid particle when the mass concentration of bismuth exceeded a threshold value.

The simulation result was compared with the test results to investigate the validity of the present eutectic model and to clarify the issued to be solved for more realistic modelling of the eutectic reactions.

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Soft Elasto-Hydrodynamic Lubrication Simulation by a Multi-Resolution Particle Method

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Key Words: *MPS Method, Lubrication, soft EHL, Computational Cost*

In this study, we developed a numerical method for simulating fluid lubrication [1] based on the moving particle simulation (MPS) method, which is a particle method. The overlapping particle technique (OPT) for the multi-resolution simulation of particle methods [2] was improved by applying an implicit algorithm to a viscosity calculation. Additionally, OPT was applied to the developed method to reduce the required number of particles and computational time. The implicit algorithm for the viscosity calculation eliminates the restriction in the time increment due to the diffusion number. In addition, we enabled the particle size to be changed significantly between sub-domains in the OPT. As a result, the pressure obtained by the developed method agreed well with the semi-theoretical solution of the Reynolds equation. The computational time of the developed multi-resolution simulation was significantly shorter than that of a single-resolution simulation.

Moreover, we developed a soft elasto-hydrodynamic lubrication (EHL) simulation method [3] based on the MPS method and OPT. In the soft EHL method, the viscosity does not depend on the pressure because the latter is relatively low. The elastic deformation of a cylinder was simulated by solving the elastic deformation equation [4] in the MPS simulation. The surface tension and cavitation were ignored when comparing the results with the semi-theoretical solutions. The results indicated that the pressure and deformation of the cylinder obtained by the developed method agreed well with the semi-theoretical solutions. It was also demonstrated that the improved multi-resolution method reduced the required number of particles and computational time while maintaining accuracy.

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SPH Modelling of Internal Erosion in Porous Media

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Key Words: *Seepage flow, internal erosion, Smooth particle hydrodynamics, constitutive model*

Internal erosion is a common phenomenon occurring in porous media caused by seepage water flow. When this phenomenon occurs, fine particles are removed from the porous media, causing significant changes in properties of porous media, including a reduction in the shear strength, an increase in compressibility and hydraulic conductivity. Consequently, the stability of geoengineering applications and adjacent structures are significantly affected. Therefore, predicting the occurrence of internal erosion in porous media is very important. In this study, an innovative smooth particle hydrodynamics (SPH) computational framework is proposed to predict the occurrence of internal erosion and its effects on the stability of geoengineering structures. In this framework, the porous media is represented by a set of Lagrangian material points, which consists of five phases, including a stable solid skeleton, erodible fine particles, fluidized particles, water, and air. Governing equations are then developed for these five phases based on the mixture theory. The mechanical response of soil during the internal erosion process is captured by a robust suction/erosion dependent softening constitutive model. The proposed framework is first employed to predict the behaviour of the classical 1D consolidation in order to demonstrate its capability in dealing with coupled flow-deformation problems. Subsequently, different erosion tests are conducted to exam the capability of the proposed modelling framework in capturing the effect of internal erosion on the mechanical and hydraulic responses of the soil structure. Comparisons between the predicted results and data available in the literature testify to the accuracy and robustness of the proposed frameworks. More importantly, the proposed framework is able to predict the entire internal erosion process, from particle separation to large deformation and failure of geoengineering structures, which demonstrates that this framework is an efficient tool to solve erosion problems that are normally difficult to be tackled by traditional mesh-based methods.

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The Meaning of Moving Particle Simulation for Gas Flow in Olfactory Display

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Key Words: *Olfactory display, Aroma gas, Multi-phase flow, MPS(Moving Particle Simulation)*

The authors have developed olfactory displays which offer scent to a user [1[[2]. In olfactory displays the controlled air flow transfers aroma gas to the nose of an user as shown in Figure 2.

The authors are computing the above 2 phased flow (aroma gas and air) by Moving Particle Simulation (MPS) in order to design and improve olfactory displays.

The authors will present the reason why they compute and simulate such 2 phase flow (aroma gas and air) by Moving Particle Simulation.

The reason and meaning of Moving Particle Simulation will be discussed by the mathematical theory of partial differential equations and the derivation of fluid dynamics (Macro-scopic) from the molecular dynamics (micro-scopic) for gas flow.

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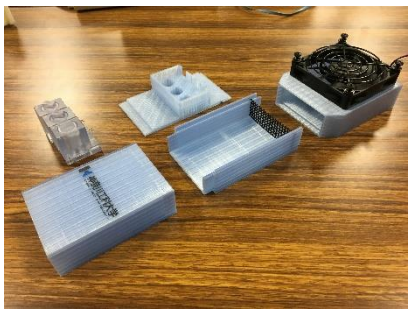

Figure 1 : Photograph of Olfactory Display

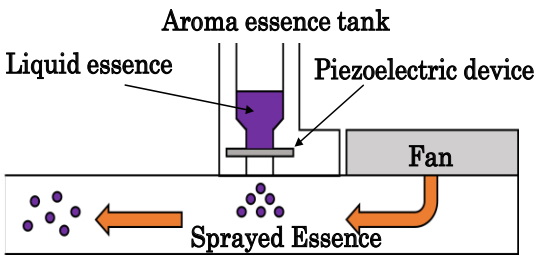

Figure 2 : Concept of An Olfactory Display

Tsunami Simulation by a 2D and 3D Coupled Multi-Resolution Particle Method

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Key Words: *MPS method, Overlapping Particle Technique, Tsunami, Computational Cost*

In this study, a two- and three-dimensional coupled multi-resolution particle method was developed based on the moving particle semi-implicit method [1] and overlapping particle technique for the multi-resolution simulation of the particle method [2], to reduce the computational cost of a tsunami simulation. By coupling the sub-domains, the developed method resolved the three-dimensional phenomena near a coastal structure in a three-dimensional subdomain and the tsunami propagation far from the structure in a two-dimensional sub-domain. The reason for coupling is that the simulation cost of two-dimensional simulations is much lower than that of three-dimensional simulations. Each sub-domain had an independent spatial resolution. The two-dimensional sub-domain had vertical and horizontal coordinates. In the tsunami propagation region, a tsunami was regarded as the two-dimensional phenomenon in which a long water wave propagated toward the coast at an angle of incidence of 0°. The three-dimensional sub-domain was composed of a middle and high-resolution sub-domains. The ellipsoidal particle model [3] that enabled the use of a lower resolution in particular directions was adopted in the three-dimensional middle-resolution sub-domain to further reduce the required number of particles. Additionally, the conventional spherical particle model was used in the three-dimensional fine-resolution sub-domain.

A tsunami was simulated using the developed method, and the wave pressures acting on the front and back walls of a coastal structure were validated. Results revealed that the wave pressures acting on the structure obtained by the present method agreed with the experimental values. It was also confirmed that the present method was effective in reducing the computational cost of the tsunami simulation by the particle method.

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A GPU-accelerated SPH method for modeling wave breaking problems

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Abstract: Smoothed particle hydrodynamics (SPH) is a meshless method with Lagrangian characteristics that is suitable for modeling incompressible flows with free surfaces [1-2]. However, the conventional SPH is limited by its low computational efficiency so that it poses great challenges for SPH to perform large-scale simulations. In this paper, we present an improved SPH method based on Graphics Processing Unit (GPU) through multi-threading to enhance the computational performance in terms of efficiency and scale. In addition, a repulsive force model that is similar to the Lennard–Jones (L–J) force is applied to avoid the particles from penetrating the boundary. The regular wave making is first used to validate the accuracy of the present GPU-based SPH method. The result indicates that the present method can achieve simulation results in good agreement with the reference data. Further, both 2D and 3D wave breaking examples are simulated by the GPU-based SPH method while the computational efficiency is discussed in depth. With the well-validated method, we numerically simulate various large-scale wave breaking problems and illustrate some underlying physical governing mechanisms.

Key Words: *Smoothed particle hydrodynamics (SPH), Graphics processing unit (GPU), Wave breaking*

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A novel Riemann solver based FPM for solving weakly compressible flows

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Key Words: *Finite particle method (FPM), Riemann solver, Weakly compressible flows, High-order accuracy*

Weakly compressible SPH (WCSPH) method developed by Monaghan [1] has been widely applied for solving hydrodynamic problems. Although the conventional WCSPH method is a simple and frequently-used approach, it is generally affected by the poor accuracy and sometimes spurious oscillations which may lead to numerical instability.

In order to dampen the pressure oscillation without introducing excessive dissipation, a modified Riemann solver with a low-dissipation limiter was proposed by Zhang et al. [2] (i.e., Riemann-SPH). The present paper aims to integrate this low-dissipation Riemann solver into the finite particle method (FPM) proposed by Liu et al. [3] to produce a Riemann-FPM which is expect to obtain better accuracy together with low dissipation.

Figure 1 shows the comparison of the pressure profile along the diagonal direction obtained by the proposed Riemann-FPM and the Riemann-SPH. It is clear that the proposed Riemann-FPM is superior to Riemann-SPH in producing smooth and accurate pressure field..

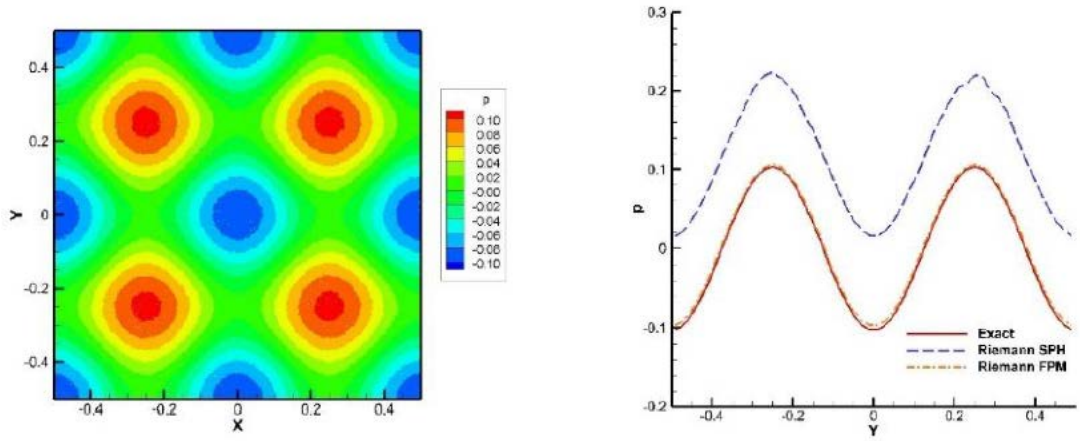

Fig. 1 Pressure profile obtained by the Riemann-FPM with dp=L/200.

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15th World Congress on Computational Mechanics (WCCM-XV)
8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII)
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A Weakly Compressible SPH Model for Modeling Poroelastic FSI Problems

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Key Words: SPH, porous media, FSI, fluid channel

We present a weakly compressible smoothed particle hydrodynamics (SPH) model, which can be applied to model the fluid-structure interaction (FSI) problems of porous media with large deformations. Two types of SPH particles, namely solid and fluid particles, are used to discretize the corresponding phase of materials. The interaction forces between the phases are derived from the theory of mixture, which is in line with the view of continuum mechanics. To stabilize the numerical scheme, the so-called $\delta-$SPH method is employed in cooperation with the artificial stress technique. The numerical model is first verified by solving a static problem: an infinite long porous medium submerged in hydrostatic conditions [1]. Then, dynamic problems, like porous structures in a fluid channel, are also investigated. In this talk, we also present a stress-based failure model in cooperation with the proposed SPH model, which can successfully reproduce the loss of material induced by the sloughing of the fluid. The new SPH model presented in this talk has a great potential to be applied in studying biomedical problems, such as biofilms or tissues' detachment in the bio-fluid environment.

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Better Vertical Stirred Milling to Help Fight the Climate Crisis

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Key Words: *Discrete Element Method (DEM), Vertical Stirred Milling, Optimisation*

Over half of all products sold globally are powders, are formed from granular or powdered material, or include at least one size reduction step as part of the manufacturing process [1]. So many products in fact, that milling and comminution contributes around 2% of global energy use [2]. However, the vast majority of that energy is wasted as heat and noise, so a better understanding and improved efficiency of this sector will help contribute towards fighting the global climate emergency.

The research presented will centre around vertical stirred milling, a continuous wet milling technique which can produce fine particles with a better energy efficiency than other types of ball mill [3]. For this reason, it is used in multiple industries, including Fast-Moving Consuming Goods (FMCG), pharmaceuticals, cosmetics and food processing. While the technology has been around for nearly a century [4], there is still a disconnect of knowledge between industry meeting particle size specifications and increased process efficiency. To bridge this gap, the Discrete Element Method (DEM) has been used so far to create, validate and simulate the behaviour of a mill under different parameters, with the aim being to find an idealistic set of operating conditions which can later be re-validated through experimentation. In future work, the simulative aspects will be extended by introducing CFD-DEM coupling, with the ultimate objective being the creation of an optimised and validated DEM simulation that can mimic the coupled properties. In turn, this reduces the amount of computational expense required; a key requirement when applying these methods to industry, where processing speed and accuracy are essential.

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Construction of a Meshfree Particle Method based on Fulfillment of Requirements on Spatial Discretization Schemes

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Key Words: *Requirements Spatial Discretization Schemes, Meshfree Particle Methods, State-based Peridynamics*

Meshfree particle methods have been considered a big promise in numerical simulation for years. Due to their enormous flexibility, arbitrarily large deformations can be handled in a Lagrangian description of the underlying differential equation. This property especially facilitates the simulation of processes with very large deformations and free surfaces, such as in the context of additive manufacturing [1] or machining operations [2].

Due to the non-unique subdivision of the domain into regular geometries and the loss of information of the direct neighbors, new challenges arise. For meshfree particle methods to accurately approximate the solution of the differential equation, numerous conditions regarding consistency and stabilization must be met [1].

For this reason, all necessary conditions on meshfree particle discretization schemes are presented. Moreover, it is shown which criteria are not fulfilled by standard meshfree particle methods like Smoothed Particle Hydrodynamcis, the correspondence formulation of state-based Peridynamics [3], [4] or the Optimal Transportation Meshfree Method. Unlike the first two schemes, the last method is based on dividing the domain into two types of points. This creates additional challenges.

Based on the aforementioned list of requirements, a new formulation based on state-based Peridynamics is presented which fulfill the necessary conditions. Several examples demonstrate the improved behavior of the new approach.

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Coupled Lattice Boltzmann-Discrete Element method for particles settling in a Bingham fluid

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Key Words: *Lattice Boltzmann Method, Discrete Element Method, Particles Sedimentation, Bingham fluids*

In this study, a coupled numerical method based on Lattice Boltzmann Method (LBM) and Discrete Element Method (DEM) is used to simulate particles settling in a Bingham fluid. The multiple relaxation time (MRT) LBM is employed to solve Bingham fluids flows[1], while the DEM is used to model particles dynamics. The coupling framework is achieved by using an immersed moving boundary technique[2]. The LBM-DEM framework is validated by simulating Bingham fluids flow around a fixed and moving cylinder (or particle). It is demonstrated that the present method can provide the accurate and efficient numerical results. Moreover, the mechanical interaction and kinematic behavior of particles are also studied, and the drafting, kissing, and tumbling (DKT) behaviors of particles are observed in Bingham fluids. The results show that the yield stress of Bingham fluids makes the drafting, tumbling and separating movement of particles more difficult.

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Modelling Particle Entrainment and Spattering in Powder-based Laser Additive Manufacturing

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Key Words: *Semi-resolved VOF0DEM, Entrainment and Spatter, Additive Manufacturing*

Particle entrainment and spattering are commonly-seen phenomena in powder-based laser additive manufacturing if laser's powder density is sufficiently high. They simultaneously evolve with the molten pool and the vapor jet, and have significant impacts on the final quality of the printed product. However, present modelling framework of massive particulate flows, unresolved CFD-DEM, demands the CFD grid size to be at least 3 times larger than the particle diameter so as to properly estimate the background fluid field. This handicaps the modelling of particle melting and deformation in Additive Manufacturing. Recently, we proposed a semi-resolved CFD-DEM that allows the mesh to be refined by employing a kernel function to reconstruct the background field [1]. In this work, we extend this semi-resolved modelling approach to Volume of Fluid method, couple recoil pressure, Marangoni Effect and other multi-physics models [2], and finally establish an Additive Manufacturing modelling framework based on semi-resolved VOF-DEM. With this model, phenomena like particle spattering and entrainment are simultaneously reproduced with molten pool evolution for the first time. Hence, it is believed that this model will be a powerful tool for future numerical investigations in various particle-fluid interactions in powder-based additive manufacturing

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Numerical modelling of concrete structures under the impact and blast loading using the smoothed particle hydrodynamics (SPH) method

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Key Words: Smoothed particle hydrodynamics (SPH), concrete, dynamic response, damage analysis

The dynamic failure process of concrete structures under the impact and blast loading can be often observed in field of military and civil engineering, which involves strong non-linear phenomena with high speed, high temperature, high pressure, high strain rate and large deformations. In this case, some typical damage and failure phenomena are difficult to be accurately reproduced by conventional methods. As a Lagrangian particle method, SPH has natural advantages in treating large material deformations in explosion and impact problems, especially in describing crack propagation of solid materials. In this work, the concrete constitutive model is added to the improved smoothed particle hydrodynamics (SPH) method. With the present novel SPH model, two validations examples are tested and analyzed. One is concrete slabs under impact loading of the steel projectile, where the entire penetration process is well modeled with different initial velocities of projectiles being considered. The other is the explosion in concrete. Two different burial depths are employed in this example and the concrete heave, throw, splash and other characteristics are well reproduced. The damage accumulation and progressive failure process are also captured by our simulation. By comparing present numerical results with the reference data, we demonstrate that the improved SPH is effective for modeling various impact and explosive problems involved with concrete structures. With the improved SPH method, the crack propagation and the damage evolution are analyzed and studied. Furthermore, it can be applicable to shaped charge jet problem and we model the whole process of shaped charge jet from detonation to penetration of target plates well while illustrating some important mechanisms, which can give guidance to the design of the shaped charge jet and protective armours.

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A cell-based smoothed finite element method for dynamic analysis of rotating plates

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Key Words: *Cell-based smoothed finite element method, Rotating plates, Mindlin plate theory, High-order rigid-flexible coupled model*

Abstract: A cell-based smoothed finite element method (CS-FEM) is formulated for dynamic analysis of a plate attached to a rigid rotating hub. The first–order shear deformation theory which is known as Mindlin plate theory is used to model the plate. Considering the high-order terms of non-linear coupling deformation which means the in-plane longitudinal shortening terms caused by transverse deformation, the high-order rigid-flexible coupled (HOC) dynamic model is established via employing Lagrange's equations of the second kind. In the process of formulating the system stiffness matrix, the discrete shear gap (DSG) method is used to construct the strains to overcome the shear locking issue. This model can not only deal with thin plate problems but also thick plate problems. The effectiveness of the CS-FEM is first demonstrated in some static cases and then extended for dynamic analysis of a rotating rectangular plate undergoing large overall motion. The simulation results are compared with those obtained by using first-order approximation coupled (FOAC) dynamic model and zero-order approximation coupled (ZOAC) dynamic model, which shows the ZOAC dynamic model can only be applied to the case with low rotating speed, and the HOC dynamic model is more accurate and has wider scope of application. The results of CS-FEM are also compared with those other existing method including the finite element method (FEM) and the assumed modes method (AMM). It is found that the CS-FEM based on Mindlin plate theory provides more accurate and "softer" solution compared with FEM even if using coarse meshes.

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A Multiscale Gradient Smoothing Method for Elliptic Problems with Heterogeneous Coefficients

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Key Words: Gradient Smoothing, Multiscale Finite Element Method, Heterogeneous Coefficients

In this presentation, we study gradient smoothing methods with improved convergence behaviors for high-contrast problems such as the flow in heterogeneous porous media. We propose a gradient smoothing method in which a smoothed gradient field within each element is constructed by utilizing the gradient fields of the adjacent elements [1, 2]. The proposed gradient smoothing method is adaptive to the heterogeneity of the problem in the sense that gradient smoothing is applied inside each of homogeneous regions separately. In addition, we propose a multiscale variant [3] of the proposed gradient smoothing method, which results in an accurate numerical solution even if a computational grid coarser than the scale of the heterogeneity is utilized. While existing gradient smoothing methods have stiffness matrices with larger bandwidth than the standard finite element method in general, the proposed multiscale gradient smoothing method has the same bandwidth as the plain multiscale finite element method. Hence, the online computational cost of the proposed method is essentially the same as that of the plain one. Improved performance of the proposed methods is demonstrated through various numerical examples.

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An adaptive edge-based smoothed finite element method (ES-FEM) for phase-field modeling of hyperelasitc materials

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Key Words: *Instructions, Multiphysics Problems, Industrial Applications, Covid-19*

Nonlinear elastomers like rubber-like polymers have been widely used by virtue of their outstanding performance. The prediction of their fracture behaviour or failure is of great significance for engineering applications and academic research. In this regard, this study presents the Griffith-type phase-field formation [1, 2] at large deformation in the framework of adaptive edge-based smoothed finite element method (ES-FEM). Thanks to the high accuracy and mesh distortion insensitivity of ES-FEM [3-5], the advantages of the phase field approach in dealing with complex cracks are sufficiently released in terms of large deformation. However, albeit the combination of the two methods manifests high precision, faster convergence rate and better robustness than existing approaches, it was testified as computationally demanding. For this reason, a multi-level adaptive mesh scheme designed for the coupling of ES-FEM and PFM was presented. Unlike the adaptive grid in the context of FEM, adaptive ES-FEM requires to identify the connectivity of the edges and their supporting elements after each update of the mesh. Notwithstanding this strategy adds about 1%~2% extra computational overhead, it not only improves accuracy but also raises computational efficiency by roughly 20 times. In addition, we also outlined the specific numerical implementation of the proposed method, the effectiveness of which is verified by several representative numerical examples. Particularly, an experiment in which cracks deflected in rubber-like solid due to impinging on a weak interface was first reproduced by our approach.

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Application of Edge-based Smoothed Finite Element Method to Large-scale Electrodeposition Simulation for Automobile Manufacturing Lines

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Key Words: Smoothed Finite Element Method, Parallel Computing, Overset Mesh Method, 4-Node Tetrahedral Meshes, Superlinear Mesh Convergence Rate, Electrodeposition

Electrodeposition (ED) [1] is widely used as an anti-corrosion base-coating method for various metal products such as automobile carbodies. In the cationic ED coating, the coating objects (cathodes) are dipped in a paint pool with electrodes (anodes), and direct current is applied from the anodes to the cathodes. Therefore, the governing equation in the space of the ED simulation is a simple Laplace equation. By calculating the time histories of electric current density at any location on the carbody surface, the distribution of deposited film thickness at the end of the ED process can be predicted. In order to guarantee a certain thickness of coating film over the entire surface, ED simulation has become an indispensable technology in automobile manufacturing.

In contrast to the computational fluid dynamics (CFD) simulation of carbodies, an ED simulation requires a meshing on complex narrow spaces in the carbody, such as side-sill. Accurate prediction of the film thickness necessitates accurate calculation of the current that passes through many small holes on the carbody surface. Therefore, the number of meshes for ED simulation is tens of millions per carbody, which requires large-scale computation. Moreover, it is necessary to handle the moving boundary using the overset mesh method because the carbodies move in the paint pool of the actual manufacturing line.

In this study, we develop an in-house ED simulator based on the smoothed finite element method (S-FEM) [2]. The edge-based S-FEM using 4-node tetrahedral meshes (ES-FEM-T4) is adopted for the BVP solver as ES-FEM-T4 has the superlinear mesh convergence rate. The MPI/OpenMP hybrid parallelization method is introduced to our code for large-scale analyses. The MINRES method is adopted for the matrix solver as MINRES can solve positive indefinite matrix equations that appear when the MPC of the overset mesh method is satisfied by the Lagrange multiplier. Our benchmark tests reveal that our simulator using ES-FEM-T4 presents much more accurate results than FEM-T4 with the same CPU time.

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Bi-directional evolutionary structural optimization of structures with gradient elasticity based on smoothed finite element method

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Key Words: Smoothed Finite Element Method (S-FEM), Bi-directional Evolutionary Structural Optimization (BESO), Gradient Elasticity, GRADELA, Stress Criterion

In this work, a structural topology optimization scheme with size effect is investigated based on Aifantis's strain gradient elasticity theory. The domain is discretised with arbitrary polygonal elements to avoid the checkerboard pattern and the essential matrices are computed using the cell-based smoothed finite element method (CS-FEM). The stringent requirement of C^1 continuous element is circumvented by employing the Ru-Aifantis theorem [3]. The main idea of the CS-FEM is to divide the element into simplical sub-cells and then use a weight/smoothing function to obtain the smoothed gradients [1]. S-FEM has the following notable characteristics: (a) does not require an explicit form of the shape functions, (b) alleviates the need of isoparametric mapping. Recently, the variant S-FEMs, cell-based, edge-based and node-based S-FEM, have been successfully incorporated in the context of structural topology optimization within the solid isotropic material with penalization method (SIMP) [2]. They proposed the smoothing domain-wise density-based method with the power-law and thus the design variables were implemented on each smoothing domain. For structural topology optimization, von Mises stress is minimized by bi-directional evolutionary structural optimization (BESO) scheme based on stress criterion that the non-local stress is obtained by the split fourth-order constitutive law on each smoothing domain. A series of numerical examples shows the effectiveness of the proposed approach.

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Implementation of the Smoothed Finite Element Method by the Complex-step Derivative Approximation

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Key Words: *Smoothed Finite Element Method, Hyperelastic Material Model, Strain Energy, Numerical Differentiation. Complex-step Derivative Approximation.*

We present a robust and efficient numerical approximation of the internal force vectors and the element stiffness matrices of the smoothed finite element method (S-FEM) [1] for a hyperelastic material model. This method is based on the complex-step derivative approximation (CSDA), which can compute first-order derivatives with high accuracy.

In this method, CSDA is used to compute internal force vectors from the computation code of the strain energy using the smoothed deformation gradient tensor. The accuracy of this method is almost the same as that of the analytical implementation. Then, based on the above results, the element stiffness matrices are computed from the strain energy using second derivatives by implementing the complex-step approach [2]. Since this method does not require the derivation and coding of analytical solutions for internal force vectors and element stiffness matrices, the complexity of implementing S-FEM is significantly reduced.

To verify the efficiency of the proposed method, it was applied for the implementation of the edge-based/node-based selective smoothed finite element method (ES/NS-FEM) [3]. In the proposed scheme, the strain energy at each integration point was computed using the smoothed gradient tensor that was reconstructed with the deviatoric deformation gradient tensor based on ES-FEM and the volumetric part of the deformation gradient tensor based on NS-FEM. This investigation confirmed that the results of the deformation and the convergences of the S-FEM are almost the same as the analytical implementation results.

Moreover, the present scheme of ES/NS-FEM was applied to the dev/vol coupled material model, which was difficult with the conventional formulation [4]. The analysis confirmed a reduction in the volume locking of the dev/vol coupled material model and the quadratic convergence of S-FEM.

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Finite Line Method for Solving Thermal Mechanical Problems

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Abstract. In this paper, a complete new collocation type numerical method, Finte Line Method (FLM), is proposed for solving general engineering problems governed by second or high order partial differential equations with proper boundary conditions. The method is based on the use of a cluster of lines crossing the collocation node under consideration and the Lagrange interpolation formulation is used to construct the shape functions over each line. When the number of the crossed lines exceeds what requires, the Least-Square technique is applied to all lines' equations to form an equation set to solve the first and high orders of partial derivatives of any physical variables with respect to the global coordinates. Then, the derived spatial partial derivatives are directly substituted into the governing partial differential equations and related boundary conditions to set up the system of equations with physical variables, temperatures and displacements, at all collocation nodes as unknowns. As an application, the proposed method is used to solve the heat conduction and mechanics problems and a numerical example is given to verify the correctness of the proposed method.

Keywords: Finite Line Method, Cross-Line Method, Heat Transfer, Mechanics.

A Couple Finite Volume and Material Point Method for Two-Phase Simulation of Liquid−Sediment and Gas−Sediment Mixtures

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Key Words: *Granular Materials, Multiphase Flow, Material Point Method*

Mixtures of fluids and granular sediments play an important role in many industrial, geotechnical, and aerospace engineering problems, from riverbed erosion and slurry flow in pipelines (liquid–sediment mixtures) to dust kick-up below helicopter rotos (gas–sediment mixtures). These mixed flows often involve bulk motion of hundreds of billions of individual sediment particles and can contain both highly turbulent regions and static, non-flowing regions. This breadth of phenomena necessitates the use of continuum simulation methods, such as the material point method (MPM), which can accurately capture these large material deformations while also tracking the Lagrangian features of the flow (e.g., the granular surface and elastic stresses).

Recent works using two-phase MPM frameworks to simulate these mixtures have shown substantial promise [1–3]; however, these approaches are hindered by the numerical limitations of MPM when simulating pure fluids. In this presentation, we present an improved, two-phase continuum simulation framework that uses the finite volume method (FVM) to solve the fluid phase equations of motion and MPM to solve the solid phase equations of motion. This numerical method is shown to accurately predict solutions to standard poromechanics problems, improve accuracy in simulations of dynamic liquid–sediment flows, and provide a robust framework for simulating gas–sediment mixtures, including rocket exhaust impinging on Martian soil.

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A Locking-Free Variational Multiscale Meshfree Formulation for Reissner-Mindlin Plate Problems

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Key Words: *Reproducing kernel particle method, Stabilized nodal integration, Variational multiscale method, Shear locking, Reissner–Mindlin plate*

The Reissner-Mindlin plate formulation in the thin-plate limit will encounter the well-known shear-locking phenomenon that must be overcome. The meshfree nodal integration can easily handle the locking issue, but it may suffer from zero and low energy instability. Although the conventional domain-subdivision-based or nodal gradient-based stabilization can avoid the low energy instability, the stabilization may cause the violation of the bending exactness (BE) in the Galerkin framework or fail to suppress the instability in the shear terms. In this research, a variational multiscale approach [1] is employed for the proposed meshfree Reissner-Mindlin plate formulation, where the solution is decoupled into coarse-scale and fine-scale under the variational equation. The coarse-scale solution utilizes the mesh-free reproducing kernel particle method (RKPM) with the stabilized conforming nodal integration (SCNI). The RK approximation in second-order monomial basis stratifies the Kirchhoff mode reproducing condition (KMRC), and SCNI guarantees the bending exactness in the Galerkin meshfree equation [2] without triggering zero-energy instability. The fine-scale solutions represent the residual of the coarse-scale equation, and the embedment of the fine-scale solutions in the coarse-scale system results in a residual-based stabilization, which eliminates the spurious oscillatory modes. The stabilization parameter is determined by dimensional analysis, and a smoothed divergence operator is applied in the fine-scale terms to ensure the satisfaction of locking free condition. RKPM naturally avoids computational challenges associated with low-quality meshes, allows efficient adaptive refinement, and provides flexible control of continuity and locality in numerical approximations [3]. The proposed framework, termed VMS-RKPM, is verified by different numerical examples, and it exhibits a better convergence rate than the conventional approach with comparable efficiency [4]. We recently developed a bending consistent nodal integration that bypasses the use of smoothing cells to enhance the efficiency, which will also be demonstrated in this study.

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A Variationally Consistent Material Point Method for Large Deformation Problems

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Key Words: *Material Point Method, Variationally Consistent Integration, Reproducing Kernel/Moving Least-Squares Approximation*

The material point method (MPM) [1] suffers from low accuracy and convergence rates compared to other meshfree numerical methods due to the under integration: the locations of material points are determined independently from the background grid and are thus suboptimal locations to perform numerical quadrature. Such an approach enables MPM to model large deformation but it also results in the loss of Galerkin exactness in the variational equation. In this research, we present a modified MPM formulation that recovers first order Galerkin exactness by employing an assumed strain variationally consistent integration method [2]. Using this approach, the gradient field of the test function space is constructed such that the numerical integration scheme is capable of numerically integrating the divergence equality, the integration constraint to achieve linear exactness. The Reproducing Kernel or Moving Least-Squares (RK/MLS) approximation [3] is introduced which overcomes the cross-cell instability because of the higher order continuity employed. The stabilization technique under the proposed integration framework is considered to remove the numerical oscillation. The proposed method is validated by solving a series of benchmark problems, and the results demonstrate that the new method can effectively improve the accuracy from the conventional MPM.

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A viscosity enhanced peridynamic model for shock wave problems

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Key Words: *Peridynamics, Shocks, Oscillatory instability, Zero-energy mode, Bulk viscosity*

The computational methods for shocks modeling demand two critical capabilities: 1) to model the dynamic fracture and fragments and 2) to capture the intermittent wave propagation. Peridynamics (PD) adopts the integral form of governing equation thus shows great advantages in modeling dynamic fracture and fragments. However, the propagation of intermittent wave within the PD based numerical system often encounters oscillatory instability. It can be attributed to the instability in time domain and the zero energy mode. To address these issues, the viscosity enhanced PD model is proposed for stabilization. The general framework is established with the introduction of artificial viscosity. Under such framework, the formulations of viscosity are developed based on the features of the spurious oscillations and improved with the balance between oscillation suppression and shock front width control. The case studies indicate that the proposed methods show good performance in shocks modeling and are well-suited for the bond-based as well as the state-based PD scheme, with which both the suppression of oscillation and control of shock front width are achieved.

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An Immersed RKPM with Transformed Interface Method for Modelling Heterogeneous Materials

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Key Words: *Immersed Methods, Meshfree Methods, Reproducing Kernel Particle Method, RKPM, Transformed Interface Method, TIM, Heterogeneous Materials*

A vast array of engineering problems involving such things as composites and biological structures require the accurate and efficient simulation of heterogeneous materials. Typically, these simulations utilize the finite element method with a body-fitted mesh in which the discretizations of two different materials conform to their interface allowing for jumps in strain or stress as one passes from one material to the other. Constructing such meshes, however, can be quite time-consuming especially for complex, three-dimensional geometry, and thus, immersed methods [1] which can work with unfitted meshes are desirable. However, immersed methods which enforce compatibility using an interfacial constraint use contour integrals over the material interface, a potentially tedious procedure given the higher-order quadrature necessary and one which often yields an ill-conditioned system due to the near-zero internal energy in the overlapping region. Furthermore, immersed methods that use a volumetric constraint in the overlapping region to impose compatibility can produce spurious oscillations and large errors in strain and stress near the interface [2].

An immersed formulation using Nitsche's method to enforce the interfacial constraint is transformed by integration by parts into a formulation which uses only domain integrals and is proposed to avoid the use of tedious contour integrals and ill-conditioned systems of the standard interfacial constraint, on the one hand, and the spurious oscillations and errors near the interface of the volumetric constraint, on the other. The resulting formulation is termed the Transformed Interface Method (TIM). Being based on a set of scattered points and capable of higher levels of continuity, meshfree methods such as the reproducing kernel particle method (RKPM) are particularly well-suited to deal with the presence of the resulting second derivative terms as well as the body-unfitted nature of immersed methods. Numerical examples are given which show the advantages of the proposed formulation.

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Application of Meshless Method in Underwater Acoustics to Solve the Back Calculation of Cavitation Tunnel Sound Source

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Key Words: *Inverse Problem, Underwater Acoustics, Reproducing Kernel Particle Method*

Underwater Acoustics positioning is an important area of research and has numerous applications. Due to the complex and variability of underwater acoustic environment, the acoustic waves may travel through extremely complex paths, which brings certain challenges to underwater acoustic positioning technology. In this research, we focus on the wave source identification in the cavitation tunnel located in National Taiwan Ocean University. According to the wave traveling distance, the wave characteristics is divided into short wave length and long wave length according to the room-size and frequency ratio. For the short-wave length, we first assume that under the condition of free field, the relationship between a point source and the resultant pressure history on a surface of a control volume surrounding the point source can be established simply by using the beam tracing method [1]. Then the surface can be considered as an equivalent source object, and any location outside the control volume can be treated as a downstream location. Similarly, in the cavitation tunnel, a carefully selected cross-section of the tunnel, which is separating the testing object and hydrophone array can also be seen as the equivalent source surface. To handle the effect of reflection, we proposed using the image source surface method (ISSM) to mimic the reflecting boundary in the cavitation tunnel. Then we use the hydrophone signals as measured data to back calculate pressure field of random upstream equivalent source surface using proposed method. The algorithm will use bisection iteration method to find the surface with the highest signal strength. For the long wave length, we solve the three-dimensional inverse Helmholtz problem [2]. The complex domain is discretized by the reproducing kernel particle method (RKPM). The RPKM method can use high order approximation and special enrichment functions to ensure the high accuracy of the solution. The numerical test shows that proper support of the kernel function should be selected for specific wave length to achieve optimum solution of the inverse problem. To test the applicability of our proposed algorithm, we first compare the result obtained from the numerical tank. The developed algorithm can successfully locate the wave source with long- and short-wave length. The developed code will be applied in the real experiment in the cavitation tunnel by the end of 2022.

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FFT-accelerated Computation for Reproducing Kernel Particle Method

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Key Words: *Meshfree, fast convolution, Fourier transform, large-scale computation*

Meshfree methods have been developed over the past few decades to overcome the limitations of the finite element method, especially when solving problems that involve major topological changes such as large deformation, fracture, flow, etc. Reproducing kernel particle method (RKPM) is a pioneer meshfree method, which uses reproducing kernel approximations and the Galerkin weak formulation to discretize the field equations. The computational cost of RKPM is however expensive, especially in 3D. Most of the efficient implementations of RKPM require neighbour search and storage, and also performing quadrature for each pair of neighbour nodes to obtain the stiffness matrix. The RK shape functions themselves are also expensive to construct since they require computing the moment matrix for each node by looping over its neighbour, and then inversing the moment matrices which have the minimum size of 4 by 4 (in 3D) [1].

Peridynamics is a nonlocal extension of continuum mechanics where spatial derivatives are replaced with volume integrals, allowing for emergence and evolution of discontinuities in the field variable, making the theory suited for fracture and fragmentation. Similar to RKPM discretization, PD simulations are computationally expensive in 2D and 3D due to the pairwise interactions of neighbouring nodes and the quadrature over the neighbourhood of each node [2]. Recently a fast convolution-based method (FCBM) for peridynamics has been introduced where the convolutional structures of PD volume integrals are exploited to allow for computing integrals via fast Fourier transform, i.e., FFT-accelerated convolution summations [3,4]. FCBM avoids explicitly identifying neighbours and looping over them for quadrature by transferring the burden of computations to cheap multiplications in the Fourier space. While most Fourier methods require periodicity of the domain which limit the applicability of them, FCBM uses an embedded constraint (EC) approach to enforce the desired boundary conditions on arbitrary geometries. In a similar fashion, the convolutional structures in RKPM formulations can be exploited to elevate the method's performance up to several orders of magnitude.

In this work, we introduce the fast convolution-based RKPM (FC-RKPM), where the convolution sums (arising from direct nodal integration of the Galerkin weak forms) are efficiently computed using FFT, and inverse FFT operations with the complexity of $O(N\log_2 N)$, where N is the total number of nodes. No prior neighbour search and storage, and no construction and storing of the stiffness matrix is required. Our preliminary 3D results show efficiency gains as high as 3000, where computations requiring months to run on a single processor can now be carried out in a few minutes!

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Investigation of Shear-Band Evolution with Concurrent Multiscale Simulation

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Key Words: *Material Point Method, Molecular Dynamics, Smoothed Molecular Dynamics, Multiscale Simulation, Shear-Band Evolution*

Developing the multiscale numerical approaches has become a more popular research issue over the last decade because these approaches can be used to simulate and evaluate the mechanical behaviors at extreme-small scales, such as the microscale or nanoscale, in a rather shorter time. In the past, a concurrent multiscale method, smoothed molecular dynamics (SMD), has been proposed to combine the molecular dynamics (MD) and material point method (MPM) in a single framework, namely, MD-SMD-MPM [1]. MD is a discrete particle method in which an appropriate potential function is utilized to calculate the interatomic forces and describe the motion of an atomic or molecular system. In contrast, the MPM is a continuum-based particle method that is formulated based on the weak form of the governing differential equations similar to the finite element method. With the use of pure MD and MPM, a series of simulations associated with copper slopes have recently been conducted to investigate the shear-band evolution at nano- and macroscale, respectively [2]. However, the distribution of the shear bands at nanoscale is discrete and the corresponding band width is between 2- and 3- particle sizes, which is different from macroscale simulation with the MPM. For further investigating the shear band evolution in concurrent simulation, a series of numerical results by using the MD-SMD-MPM will be presented in this presentation.

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Nodally-integrated RKPM for modeling deposition processes in three-dimensional printing

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Key Words: *Meshfree, 3D printing, deposition, thermo-mechanical, nodal integration*

A stable and efficient nodally-integrated reproducing kernel particle method (RKPM) [1,2] is introduced in this work for effective modeling of the deposition types of three-dimensional printing that involve thermo-viscous and viscoplastic flow. Coupled mechanical and thermal effects are considered in this work. First, it is shown that nodal integration of the coupled equations results in severe spurious oscillations in the solution, worse than pure mechanical problems. A naturally stabilized and variational consistent nodal integration is then proposed for the coupled equations to stabilize the solution and provide *n*th order convergence in the two-field problem [3,4]. Generalized thermo-mechanical theories of the hyperbolic type are also leveraged for a uniform explicit critical time step, with results essentially the same as the classical theory. Benchmark problems are solved to demonstrate the effectiveness of the proposed method in obtaining stable and accurate RKPM results under both thermo-viscous and viscoplastic flow. Simulations of three-dimensional printing are presented, including fused deposition modeling, and printing of concrete.

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Particle-informed FEM: A method for accurately simulating the shock phenomenon of fiber reinforced composites

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Key Words: *Finite element method, Material point method, Fiber reinforced composites, Mesoscopic model; Impact problem; Shock phenomenon*

The fiber reinforced composites exhibit outstanding features under impact loading conditions. It is important to understand how different constituents and composite microstructures affect the meso-to-macro level mechanical performance. The finite element method (FEM) has difficulties in mesoscale modeling and failure evolution problems due to the complex microstructures of the yarn and matrix. The material point method (MPM) overcomes the aforementioned limitation and has successfully simulated the plate impact problem with glass-fiber reinforced polymer composites (GRP) [1]. However, we observe that the rising time of the stress wave on the GRP free surface is inconsistent with that of the experimental data [2], which indicates that the MPM cannot accurately describe the shock phenomenon.

In this presentation, a particle-informed FEM that can accurately describe the rising time of stress wave, as consistent with the experimental data, is proposed to better simulate the shock response of the GRP composite systems. A two-dimensional computational model of GRP is established based on the MPM mesoscopic model. The numerical simulation is performed by using the particle-informed FEM, and compared with the MPM and experimental data, which demonstrates that the particle-informed FEM can accurately describe the shock phenomenon as compared with the MPM. Additionally, the corresponding mesh convergence effect of the particle-informed FEM is also discussed.

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Phase-field Implicit Material Point Method for Finite Deformation Elastoplastic Fracture Modelling of Geomaterials

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Key Words: *Implicit Material Point Method, Phase Field, Elastoplastic Fracture, Finite Deformation*

Abstract

A phase-field implicit material point method with the convected particle domain interpolation (PF-ICPDI) is developed to model the finite deformation elastoplastic fracture behavior of geomaterials, especially in considering the brittle-ductile failure transition process. In this method, a smooth two-yield-surface plasticity constitutive model is adopted to evaluate the complex elastoplastic deformation behavior of geomaterials. To simulate the brittle-ductile failure transition process, a phase-field fracture model derived from the microforce balance law is used to couple with the cap plasticity model by introducing an effective phase-field stress. Furthermore, the implicit material point method combining with the convected particle domain interpolation technique is utilized to avoid severe mesh distortion and improve the computational accuracy in treating the quasi-static large deformation elastoplastic fracture problem. The staggered incremental iterative scheme is implemented for the solution of the coupled discrete governing equations. Numerical simulations demonstrate that the proposed PF-ICPDI method can effectively and accurately capture complex fracture behaviors of elastoplastic geomaterials. This work was supported by the NSFC (Nos. 12072062 and 12072061), the LiaoNing Revitalization Talents Program (XLYC1807193), Key Research and Development Project of Liaoning Province (2020JH2/10500003) and Fundamental Research Funds for the Central Universities (DUT20LAB203).

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Temporal Stability of Collocation, Petrov-Galerkin and Other Non-symmetric Method in Elastodynamics and an Energy Conserving Time Integration

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Key Words: Collocation, Petrov-Galerkin, Temporal stability, Elastodynamics, Non-symmetric, Energy conservation

Non-symmetric matrices may arise in the discretization of elastodynamics when a Petrov-Galerkin, collocation method, or finite-volume method is employed. While these methods have been widely applied, it will be shown that the use of these non-symmetric matrices is inconsistent with the conservation of energy in the elastodynamic problems. First, the consistency between the continuous forms of the momentum equation and energy equation is examined. It is shown that the conservation of linear momentum is equivalent to conservation of energy provided the solution is sufficiently smooth. The semi-discrete counterparts are then examined, where it is shown they are also equivalent, but only conditionally: the mass and stiffness matrices must be symmetric. As a result, employing a non-symmetric method elastodynamics may artificially generate or dissipate energy. The fully discrete forms with Newmark time integration are then examined where it is shown that unconditionally unstable algorithms may arise. An energy-conserving time integration algorithm is then proposed which provides stability non-symmetric systems. The reproducing kernel (RK) collocation and finite-volume methods are employed in numerical examples as the typical non-symmetric methods to demonstrate the effectiveness of proposed time integration methodology.

A highly efficient and accurate Lagrangian-Eulerian stabilized collocation method (LESCM) for the fluid-structure interaction problems with free surface

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Abstract: A novel numerical method for the fluid-structure interaction problems with free surface is proposed in this work. The method is based on the hybrid Lagrangian-Eulerian description. The problem domain covering the fluid is discretized into the Lagrangian particles which carry the fluid information, and the problem domain covering the entire movement space is discretized into the uniformly distributed Eulerian background nodes. The coupling governing equations of the fluid, structure and interface are solve by the meshfree stabilized collocation method employing the reproducing kernel (RK) approximation on the Eulerian nodes. The solution is very efficient since the Eulerian nodes are set to be the initial positions in each time and it's no need to reconstruct the shape function. The information mappings between the Lagrangian particles and the Eulerian nodes are also conducted by the RK approximation which can keep the mass and momentum conservation of the solution. The cell-cut algorithm is introduced to couple the fluid and the structures which can solve the fluid pressure and the fluid-structure interactional force simultaneously and avoid the complicated iterations of the traditional interaction algorithms. Several numerical examples including the collapse of water column with a rigid barrier, water entry of a half-buoyant circular cylinder and a rigid box rotating and sinking in water are simulated, which demonstrate the high accuracy, high efficiency and good stability of the proposed method. This method can be extensively applied to the engineering applications with fluid-structure interactions.

Key Words: *fluid-structure interaction, free surface, Lagrangian-Eulerian stabilized collocation method, reproducing kernel approximation, conservation, high accuracy and efficiency*

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Dynamic Phase Field Modelling of Magnetic Vortex Evolution under Elastic Wave

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Key Words: *Ferromagnetic materials ; Elastic wave; Magnetic vortex; Phase field; Nonlinear finite element*

Magnetic vortex has attracted much attention due to its potential application in magnetic logic and memory devices. Understanding the dynamic response of magnetic vortex subjected to elastic waves is crucial for its application in the future devices. In the present study, a dynamic phase field model based on the LLG equation, Maxwell equation and elastodynamic equation is proposed to predict the evolution of magnetic vortex under elastic wave. Due to nonlinearity and multi field coupling, the phase field equations cannot be solved by normal finite element method. Based on the multi-field coupled variation method, a nonlinear finite element method is employed to solve the governing equations of the phase field model. The phase field model based on finite element is able to simulate the evolution of the topological structures with complex geometrical shapes and arbitrary boundary conditions under elastic waves. In order to confine the magnetization amplitude near saturation magnetization, Lagrange multiplier method is adopted in the phase field model. The phase field simulations show that the high frequency force applied to the left side of the film produces an elastic wave of short wavelength in the film. The elastic wave can induce the reversal of vortices. The results in the present work suggest that elastic wave can be used to remotely control the topologically nontrivial vortex in ferromagnetic thin films, which may hold promise for applications in magnetic devices.

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LRBF Collocation Method for Rayleigh-Taylor Instability Under Different Gravity

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Key Words: *Local Radial Basis Function, Collocation, Rayleigh-Taylor Instability, Gravity Effect*

Rayleigh-Taylor instability is an instability phenomenon at the interface where a denser fluid is placed on the top of a lighter fluid in a gravitational field, such as in astrophysics the crab Nebula formed by an exploding supernova, and in nuclear engineering inertial confinement fusion controlled by Rayleigh-Taylor mixtures. In this paper, the local radial basis function (LRBF) collocation method is used to solve Rayleigh-Taylor instability problem. We use collocation method to avoid a time-consuming process to generate mesh. Meanwhile, different topological methods are adopted for the local collocation points to avoid problems similar to the full matrix and ill-condition of the global interpolation matrix. As a result, the positions of rising bubbles and falling spikes obtained from the calculation are compared with those achieved from literature, and a good agreement is obtained. In addition, we also analyzed the position changes of rising bubbles and falling spikes under different gravity effects. With the increase of gravity, the rate of rising bubble slows down while the rate of falling spikes basically remains unchanged, which provides a basis for future research on Rayleigh-Taylor instability in extreme environments.

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Physics-informed-based collocation solver

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Abstract: This paper introduces the recent advances on physics-informed-based collocation methods (PICM) and their various engineering applications [1-4]. The basic concepts of the physics-informed-based collocation methods are first introduced, such as the global and localized collocation schemes, physics-informed kernel functions. Introducing any underlying physical laws as prior information, a group of physics informed kernels could be derived to provide the efficient and accurate numerical solutions of PDEs in the kernel-based collocation solvers. The PICMs can be classified into two categories, namely, global physics-informed collocation methods and localized physics-informed collocation methods. Several numerical examples demonstrate the efficiency and accuracy of the proposed physics-informed-based collocation solver.

Keywords: Global collocation methods; Localized collocation methods; physics-informed kernel functions; meshless

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Evaluation of the effect of molecular chain structure and crystallinity on the mechanical properties of Polyamide by the Finite Element Method of modified MCN model

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Key Words: *polyamide, hydrogen bonding, strain rate dependence, crystallinity, constitutive equation, finite element method*

Polyamide (hereafter, PA) is a semi-crystalline polymer in which repeating units of amide groups (-NHCO-) is contained in a molecular chain. PA shows excellent mechanical properties by intermolecular hydrogen bond between hydrogen atom and oxygen atom of amide groups at neighboring molecular chains. The hydrogen bond densities and existence of aromatic ring in the molecular chain affect the rigidity of the molecular chain. In addition, the nonlinear mechanical behavior of PA is characterized by the debonding and rebonding of intermolecular hydrogen bond [1]. Predicting the mechanical properties of PAs having different molecular structures is very important to the research and development of new materials such as bio-based PA.

In this study, the effects of the tensile rate, density of amide groups and crystallinity were investigated by uniaxial tensile tests of commercial PA, PA11, PA610, amorphous/semi-crystalline PA6, and amorphous/semi-crystalline PA-MXD10. In addition, the surface of the test pieces during the tensile test were photographed, and the local strain generated in the test pieces during the tensile test was evaluated by the Digital Image Correlation (DIC) method. The mechanical response and the strain distribution significantly affected by the molecular-structure and crystallinity of PA. The initial stiffness and strength of PA increases with the density of the hydrogen bond and crystallinity. In amorphous PAs, the rapid drop of stress was observed after reaching the maximum stress whereas the stress gradually decreases in the crystalline PAs. The prominent strain concentration was observed at the necked region in the PA showing rapid stress drop. The numerical predictions of the mechanical response and strain distribution characterized by the molecular chain structure and crystallinity are important for the material development of PA.

To represent the experimentally observed mechanical characteristics of PA, the constitutive equation based on the debonding and rebonding of intermolecular chain [2] was applied for PA, and the neck propagation process under uniaxial tensile deformation was demonstrated by the numerical simulation based on the large-deformation rate-form finite element method. The simulation results reproduced the mechanical responses and development of strain distributions of several kinds of PA.

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Multilevel Adaptive Mesh Refinement with controlled accuracy for nonlinear quasi-static mechanics

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Key Words: Adaptive Mesh Refinement, Local Multigrid Methods, Nonlinear Solids Mechanics, Field Transfer, Error Control

We propose an adaptive mesh refinement (AMR) algorithm dedicated to the simulation of nonlinear quasi-static solid mechanics problems with phenomena localized at the structural scale [1]. The proposed method allows us to follow in time the evolution of studied phenomena in a *fully-automatic* (thanks to an *a posteriori* error estimator [2]), *precise* (respecting user-prescribed accuracies) and *efficient* (in terms of memory space and computational time) way.

We adopt the multilevel Local Defect Correction (LDC) refinement method [3] for its great potentialities for solving elliptic problems [4]. We propose an algorithmic extension of the LDC method to nonlinear quasi-static problems and provide key aspects associated to its practical implementation. We highlight its efficiency in the nonlinear context and show its natural ability to generate a hierarchy of meshes of limited sizes that dynamically follow the evolution over time of studied phenomena.

We address generic AMR-related questions associated to dynamic mesh adaptation, such as fields transfer between time steps as well as the discretization error control over time. We propose a straightforward and efficient equilibration strategy lying on the introduction of the initial non equilibrated residual as a source term of the problem. We also develop a reliable remeshing algorithm aiming to limit the number of mesh regeneration over time while guaranteeing the fulfillment of prescribed errors.

Several numerical experiments, in $2D$ and $3D$, with different types of material behavior as well as variable loadings are proposed to validate the efficiency of the developed algorithm.

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On the modeling of non-linear imperfect interfaces including plasticity and stochastics effects

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Key Words: Imperfect Interfaces, Plasticity, Stochastics

Gluing has become in recent years an essential technique for the assembly of structures. These techniques are even essential in aeronautical or marine engineering. Although many models are available in the literature, much work remains to obtain reliable and accurate one.
A recently developed technique in this framework uses asymptotic expansions to generate models that take into account the small thickness of adhesive joints but also finite strains or damage. Non-linear effects are often prevalent for certain adhesives used in engineering. In this talk, we will extend this technique to associated and non-associated elasto-plasticity. It will be shown that the limit problem is very close to a Coulomb friction type model.
Another very important element is the control of uncertainties due to, for example, bonding defects, thickness irregularities, the presence of micro-cracks, etc. For this purpose, we propose to work in the framework of stochastic PDEs (Ito integral). Some theoretical and numerical results will be presented during the talk.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Abstract Title

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Key Words: ensemble filtering, nonlinear hyperreduction, multi-fidelity Monte Carlo, data assimilation, uncertainty quantification, aerodynamics

We present an efficient data assimilation framework for nonlinear dynamical systems that uses multi-fidelity statistical estimates based on a projection-based hyper-reduced order model (ROM) that is trained on-the-fly. This framework is particularly applicable to conservation laws in aero- dynamics that yield expensive forward models. The formulation comprises the following technical components: (i) an ensemble Kalman filter to tractably handle high-dimensional, strongly-nonlinear dynamical models; (ii) multi-fidelity forecast models, where ROM-based coarse fidelities are con- structed on-the-fly; and (iii) hyperreduction for the ROM, based on proper orthogonal decomposi- tion and the empirical quadrature procedure, constructed using the ensemble of full order model trajectories. We show that the multi-fidelity statistical estimates based on efficient, on-the-fly construction of the ROM enables the rapid and reliable state estimation for practical nonlinear dynamical systems. We demonstrate the effectiveness of our framework to estimate the state of a separated flow around an airfoil by (i) showing that the ROM-based multi-fidelity method is more accurate than the single-fidelity method for comparable computational cost and (ii) showing that multi-fidelity statistics enable the use of a less accurate surrogate when compared against ROM-only filters at negligible cost.

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A weakly-invasive LATIN-PGD method for non-linear problems

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Key Words: Reduced-order model, weakly invasive, LATIN-PGD, non-linear, SAMCEF

Reduced-order models (ROM) are powerful engineering tools that allow reducing drastically computational time for complex problems in order to build "virtual charts" [1]. Among other ROM technics, the LATIN-PGD provides a reduced-order basis without any a priori knowledge of the problem nor snapshots and is particularly suitable for non-linear simulations [2,3]. However, the development of ROM-based methods in the industry is currently slowed down by the difficulty of introducing them into commercial finite element software, mainly due to the strong intrusiveness of the associated algorithms. This work introduces a weakly-invasive reformulation of the LATIN-PGD method [4], in the form of generalized quantities, which is intended to be directly integrated into the finite element analysis software. The main idea remains to reuse all facilities already included in an industrial solver (all non-linearities, element types, capabilities, ...) by only changing the non-linear solver algorithm. As part of this work, this approach is carried out in the non-linear finite element analysis software SAMCEF developed by Siemens. The feasibility of the method is highlighted with some particular problems: elastic-visco-plastic material, contact, parametrized aspects.

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Constructing Reduced Order Model for Two Phase Flow using Dynamic Mode Decomposition

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Key Words: *Dynamic Mode Decomposition, Multiphysics Problems, Reduced Order Model*

In developing products to achieve higher efficiency, the computational fluid dynamics (CFD) is being used. In addition to cutting costs by reducing the number of prototypes, there is a growing need for technology that reduces design time by using automatic optimization and other methods. However, since the computational cost of CFD is very high, it is difficult to apply to automatic optimization, and there is a strong need to reduce the analysis time. As a trend in speeding up CFD, constructing reduced order models (ROM) have attracted much attention in recent years. Dynamic mode decomposition (DMD)[1] is one of key techniques for identifying low-dimensional dynamic system from spatio-temporal data in numerical and experimental fluid mechanics, and has received much attention because it can be used to construct ROMs.

Although DMD has been applied to various problems, its applications to the two-phase flow analysis are limited. As previous study, Krolick and Owkes[2] presented a technique to extract the primary instability from an atomizing jet's core. In order to apply DMD to more general two phase flows, in this study, we investigated the stability of ROMs obtained by different definitions of the gas-liquid interface: the raw VOF field and a signed distance function.

The current study presents a technique to extract wave form of sloshing tank problem. The simulation was conducted using a volume of fluid (VOF) method and the experimental data by Goudarzi and Sabbagh-Yazdi[3] was used to verify the simulation result. The ROM was constructed for the flow field using the randomized DMD[4], and there is an instability issue that occurs when DMD is applied to the VOF field. The reason for this comes from the discontinuity of the VOF fields both in space and time. The current study revealed that the ROM constructed by the hyperbolic tangent function of the signed distance function gives more stable result than other definitions of the gas-liquid interface.

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Empirical Quadrature Procedure with Constraint Reduction for Reduced Order Modeling of Large Scale Problems

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Key Words: Model reduction, hyperreduction, constraint reduction, aerodynamics

Projection-based model reduction of parametrized/unsteady nonlinear partial differential equations (PDEs) requires hyperreduction to accelerate the evaluation of the reduced residual. Our approach to hyperreduction is based on the empirical quadrature procedure (EQP)[1], which solves a constrained optimization problem to identify a reduced (i.e., sparse) quadrature rule tailored for a given reduced basis and the parametrized/unsteady problem that satisfies "residual matching conditions" at a set of parameter/time training points. The selection of the training points, or more generally constraints, is crucial, and we wish to meet two competing requirements: a large number of training points to ensure that the residual is well approximated over the entire parameter/time domain; a small number of training points to reduce the training cost. These competing requirements pose challenges especially for large-scale and high-dimensional problems.

To handle these challenges, we present a rigorous and efficient approach to hyperreduction, with an emphasis on large-scale and high-dimensional problems. Our formulation exploits the fact that, in many parametrized systems, the constraints belong to a manifold, are similar, and hence are amenable to substantial reduction. We develop a constraint reduction algorithm that uses QR factorization to determine a set of orthogonalized constraints, along with judiciously selected truth values and tolerances, such that our original constraints are well represented. The factorization is used to rank the "importance" of each constraint, then an iterative process selects a minimal set of constraints, while ensuring that the resulting solution satisfies all original constraints. We exploit the powerful constraint reduction capabilities of this method to develop an algorithm for efficiently sampling a large or high-dimensional parameter space. This approach employs a greedy algorithm to rapidly determine a minimal set of training points such that the resulting reduced quadrature rule is accurate over the entire parameter domain.

We demonstrate the formulation using a family of large-scale and high-dimensional aerodynamics problems, including the following: parametrized Reynolds-averaged Navier-Stokes (RANS) flow over an ONERA wing; multi-fidelity ensemble Kalman filter for separated Navier-Stokes flow past NACA0012; and high-dimensional parametric uncertainty quantification of the RANS Spalart-Allmaras turbulence model. For these large-scale problems (up to 40,000 constraints and 10^6 quadrature points), we observe significant improvements in the training time when the constraint reduction methods are employed.

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Model Reduction for Aerodynamics: High-Dimensional Problems and Shape Optimization

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Key Words: model reduction, error estimation, adaptivity, optimization, aerodynamics

We consider model reduction of shape-parametrized aerodynamics problems governed by the Euler and Reynolds-averaged Navier-Stokes (RANS) equations. Our goal is to provide rapid and reliable predictions of quantities of interest, such as lift and drag, with an emphasis on high-dimensional problems arising from geometry parametrizations in design optimization and uncertainty quantification. The key ingredients are the adaptive high-order discontinuous Galerkin (DG) finite element method, which provides efficient solutions of convection-dominated problems; reduced basis (RB) spaces, which provide rapidly convergent approximations of the parametric manifolds; the dual-weighted residual (DWR) method, which provides effective error estimates for quantities of interest in both the DG and RB approximations; and the empirical quadrature procedure (EQP), which provides efficient hyperreduction. We consider the application of the shape-parametrized model in two distinct context.

The first is the construction of a shape-parametrized hyperreduced model and its application to probabilistic analysis under geometric uncertainties. A weak greedy algorithm simultaneously adapts the DG spaces, RB spaces, and EQP to meet the user-specified output error tolerance over the entire parameter space. The algorithm adaptively enriches the training parameter set to effective train the reduced model in high-dimensional parameter spaces. In the online stage, the DG-RB-EQP method reduces the computational time by several orders of magnitude. In the offline stage, the adaptive training algorithm provides efficient training while controling the discretization errors associated with the DG, RB, and hyperreduction approximations.

The second is in the context of aerodynamics shape optimization. We combine the above ingredients with a trust-region method to construct a sequence of reduced models on-the-fly to accelerate the optimization process. The key additional ingredients are the trust region informed by the DWR error estimate, and the tailored EQP hyperreduction which ensures that the reduced model satisfies required consistency conditions for the convergence of the trust-region method. We demonstrate on-the-fly acceleration of shape optimization procedure using an inverse-design problem and a drag-minimization problem.

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Multi-component Reduced Order Modeling Framework for Rocket Combustion Engines

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Key Words: Reduced Order Modeling, Domain Decomposition, Rocket Combustion

Combustion dynamics is characterized by the coupling between heat release, hydrodynamics, and acoustics. In combustion engines, this complex coupling can lead to combustion instabilities that can cause devastating engine failures. Even with advances in modern computational capabilities, high-fidelity (e.g., Large Eddy) simulations of full-scale engines remain out of reach. In this work, we develop a framework to enable efficient prediction of combustion dynamics in rocket engines using component-level training on reduced domains, and integrating these components as a network of Reduced Order Models (ROMs). The full rocket engine is decomposed into different components, each of which adapts different modeling strategies. Model reduction methods using model-form preserving least-squares projections with variable transformation (MP-LSVT) [1] are adapted to obtain efficient and accurate ROMs to represent complex combustion dynamics near rocket injectors. These ROMs are effectively trained based on offline LES simulations with a reduced number (e.g., < 3) of injectors, a small fraction of the full-scale engine, which usually contains hundreds of injectors. External excitation is introduced in the offline LES simulations to incorporate essential dynamics for ROM training. The trained ROMs are then coupled to form a network. Computational fluid dynamic (CFD) models are used in components, dominated by acoustically propagating waves (manifolds, injector posts, and nozzle) and coupled to the aforementioned network of ROMs which model the near-injector dynamics [2]. We demonstrate the framework to predict combustion instability characteristics in a multi-injector rocket engine.

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Nearest-Neighbor Bases for Efficient Model Reduction of Parameterized Nonlinear Dynamical Systems

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Key Words: *adaptive bases, model reduction, parametric PDEs, nearest neighbors*

Projection-based model order reduction (PMOR) techniques rely on the precomputation of an approximation subspace that, despite having a dimension much smaller than that of its underlying high-dimensional model (HDM), exhibits the ability to capture its dominant features. It is common to construct this approximation subspace by collecting many solution snapshots from the HDM and compressing a matrix of these snapshots using the singular value decomposition (SVD). However, for highly nonlinear problems that are convection-dominated or characterized by mutiple distinct scales or regimes (or more generally, any problem with a high Kolmogorov n-width), a single global reduced-order basis (ROB) often needs to be prohibitively large to deliver sufficient accuracy. One existing method [1] addresses this issue by partitioning the state space into regions with a clustering algorithm and pre-computing multiple smaller ROBs, one for each region of the partitioned state space. Then at each time-step of the simulation, the ROB constructed for the region of state space occupied by the current state vector is used to advance the simulation. This leads to a piecewise affine approximation manifold where each local ROB is constructed by compressing snapshots in the neighborhood of the current state vector, with these neighborhoods constructed a priori by a clustering algorithm.

The PMOR method proposed here similarly makes use of the concept of state-space locality, using at each time-step a ROB constructed from snapshots in the neighborhood of the current state vector. However, the proposed method discards the a priori partitioning of the state space into a discrete number of neighborhoods via clustering and the pre-computation of ROBs via data compression. Instead, at each time-step, it constructs on-the-fly a ROB using a small number of nearest snapshots to the current state vector without any data compression. Efficient distance formulas are derived to enable the real-time construction of such nearest-neighbor ROBs which by design, are adaptive. Using this approach, the offline processing of PMOR is simplified and made more computationally efficient, the dimension of the local projection-based reduced-order model needed to achieve a certain level of accuracy is made smaller than otherwise possible, and therefore the overall computational efficiency of PMOR is significantly improved. Under reasonable conditions, the proposed PMOR approach is capable of achieving a perfect accuracy for "reproduction" problems using exceedingly small basis sizes. Its potential for parametric, highly nonlinear, convection-dominated flow problems is demonstrated on several parametric, large-scale, CFD applications pertaining to aerodynamics, using the least-squares Petrov-Galerkin (LSPG) method [2] for PMOR.

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Nonlinear Projection-Based Model Order Reduction in the Presence of Adaptive Mesh Refinement

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Key Words: *adaptive mesh refinement, CFD, model reduction, hyperreduction*

For many problems in computational mechanics, Adaptive Mesh Refinement (AMR) is desirable as it enhances accuracy for a given computational cost and reduces this cost for a specified accuracy. While it is fairly practiced in the context of high-dimensional, mesh-based computational models, it is in its infancy in that of low-dimensional, generalized-coordinate-based computational models such as Projection-based Reduced-Order Models (PROMs) and Hyperreduced PROMs (HPROMs). This is primarily due to the fact that when AMR is applied at the high-dimensional level, different solution snapshots may be computed on different meshes, which raises two different but related issues: the solution snapshots may have different dimensions, which complicates their collection and compression into a Reduced-Order Basis (ROB); and even if they happen to have the same dimension due to a fortuitous balance between mesh refinement in some regions of the computational domain and mesh coarsening in other regions, they may suffer from some inconsistency due to the fact that their same-index entries may not evaluate the solution at the same spatial location. Recent work in the literature [1] addresses, to some extent, both aforementioned issues by interpreting all mesh-based computations underlying the data-driven POD procedure as inner products and computing them in the continuous solution space rather than the semi-discrete counterpart. Here, this approach is extended to hyperreduction, which is indispensable for parametric, Projection-based Model Order Reduction (PMOR) when it is not possible or computationally tractable to pre-compute offline the reduced-order operators and quantities, and the computational complexity of their online computation does not scale only with the size of the PROM. Specifically, the context is set to that of the Energy-Conserving Sampling and Weighting (ECSW) hyperreduction method presented in [2] for second-order dynamical systems semi-discretized by finite element methods, and recently extended in [3] to first-order hyperbolic problems discretized by finite volume methods. To achieve computational tractability in the presence of AMR, the concept of local ROBs in the state-space [4] is adopted. This concept is equipped with that of local "supermeshes", where the construction of each local supermesh is dictated by the subset of the collected solution snapshots underlying the construction of a local ROB; and the reduction of such a supermesh is performed and trained using the underlying local ROB and ECSW. All presented ideas and their significance are illustrated and highlighted with the solution of three-dimensional, nonlinear, convection-dominated turbulent flow problems.

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Nonlinear reduced models for parametric/random partial differential equations

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Key Words: Parametric PDEs, reduced models, piecewise polynomials, reduced basis spaces

We consider model reduction methods for parametric/random partial differential equations. The usual approach to model reduction is to construct a linear space V_n of (hopefully low) dimension n which accurately approximates the parameter-to-solution map, and then use it to build an efficient forward solver. However, the construction of a suitable linear space is not always feasible. It is well-known that numerical methods based on nonlinear approximation outperform linear methods in many contexts. In a so-called library approximation, the idea is then to replace the linear space V_n by a collection of linear or affine spaces $V_1, V_2, \ldots, V_N$ of dimension $m < n$.

In this presentation, we first review standard linear methods for model reduction before introducing nonlinear reduced models with a focus on library approximation. We then present different strategies which can be used to generate such nonlinear reduced models, namely libraries based on piecewise (Taylor) polynomials and on local reduced basis spaces. We provide some theoretical results and illustrate the performances of the methods through several numerical experiments.

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Operator inference to construct low-dimensional models for incompressible flows

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Key Words: Data-driven modeling, operator inference, reduced-order models, incompressible flows

Dynamical modeling of a process is essential to study its dynamical behavior and to perform engineering studies such as control and optimization. With the ease of accessibility of data, learning models directly from the data have recently drawn much attention. It is also desirable to construct compact low-dimensional models describing complex non-linear dynamics, leading to perform simulations and engineering studies on modest computer hardware. To that aim, the construction of low-order models is well reflected in the recent successes of data-driven approaches such as dynamic mode decomposition and operator inference. However, for a process, typically, some known physical constraints (e.g., mass conversation, energy conversation) are not incorporated in learning models using the approaches above.

In this talk, we discuss the use of the operator inference approach to learning structured low-dimensional models for incompressible flow from data. To that end, we utilize the intrinsic structure of the Navier-Stokes equations for incompressible flows and show that learning dynamics of the velocity and pressure can be decoupled, thus leading to an efficient operator inference approach for learning the underlying dynamics of incompressible flows. Finally, we show the operator inference performance in learning low-order models using some benchmark problems and compare it with an intrusive method and other data-driven approaches.

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Parameterized Neural Ordinary Differential Equations: Applications to Computational Physics Problems

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Key Words: Model reduction, autoencoder, neural ordinary differential equations

This work proposes an extension of neural ordinary differential equations (NODEs) by introducing an additional set of ODE input parameters to NODEs. This extension allows NODEs to learn multiple dynamics specified by the input parameter instances. Our extension is inspired by the concept of parameterized ordinary differential equations, which are widely investigated in computational science and engineering contexts, where characteristics of the governing equations vary over the input parameters. We apply the proposed parameterized NODEs (PNODEs) for learning latent dynamics of complex dynamical processes that arise in computational physics, which is an essential component for enabling rapid numerical simulations for time-critical physics applications. For this, we propose an encoder-decoder-type framework, which models latent dynamics as PNODEs. We demonstrate the effectiveness of PNODEs with important benchmark problems from computational physics.

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Piecewise polynomial approximation manifold for the model reduction of nonlinear convection-dominated problems

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Key Words: *CFD, hyperreduction, projection-based model order reduction, quadratic approximation manifold*

Projection-based model order reduction (PMOR) provides a parsimonious description of otherwise a very high dimensional parametric model (HDM), by constructing global shape functions as opposed to local ones – often used in the context of finite element methods. The key difference in the case of PMOR is that the global shape functions are computed based on prior knowledge of the problem to be solved, obtained through exercising the parametric HDM. The low-dimensional description of a computational model afforded by PMOR, equipped with hyperreduction in the case of an arbitrarily nonlinear model significantly accelerates the time-to-solution of the problem of interest. For example, in [1], the authors demonstrate the ability of PMOR to reduce the wall-clock time required by a turbulent flow computation past a complex geometry from 100 *hours* on over 3500 CPU cores for the HDM, to only 3 *minutes* on 32 cores for its hyperreduced, projection-based reduced order model (HPROM) counterpart. Unfortunately, for highly nonlinear problems and in particular for convection-dominated problems, the performance of traditional PMOR techniques is greatly limited by the Kolmogorov barrier which underscores the need for many basis vectors for an affine approximation to achieve reasonable accuracy. To meet this challenge, a variety of nonlinear rather than affine approximations have been proposed, from locally affine approximations [2] that have demonstrated their potential for 3D challenging applications [1], to more general nonlinear approximation manifolds generated by neural networks [2] that seem to be limited to simple 1D and 2D applications – due to the extensive training and hyper-parameter tuning they require, which questions their practicality.

Here, an alternative, piecewise quadratic approximation manifold is proposed for mitigating the Kolmogorov barrier. It is trained in a two-step approach that builds on the data-driven approach underlying the traditional construction of PROMs; is application-independent; is linearization-free and therefore is more robust for highly nonlinear problems. Most importantly, if for a nonlinear, convection-dominated flow problem a PMOR method equipped with the traditional affine approximation delivers a certain level of accuracy using a PROM of dimension n, the proposed piecewise approximation manifold produces a piecewise quadratic PROM that delivers a similar level of accuracy using however a dimension that is smaller than $\sqrt{n}$. The proposed piecewise approximation manifold is implemented in the least-squares Petrov-Galerkin (LSPG) method for PMOR and equipped with the ECSW method for hyper reduction [1]. Its superior accuracy for a fixed low dimension n and its superior performance for a fixed level of accuracy are demonstrated for several realistic, convection-dominated, turbulent flow problems.

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Projection-based Model Order Reduction of Embedded Boundary Models

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Key Words: Embedded Boundary Method, Nonlinear Model Order Reduction, Hyperreduction

The state of the art of nonlinear, projection-based model order reduction (PMOR) has significantly advanced in recent years for many applications, including computational fluid dynamics (CFD) analysis. For example, the least-squares Petrov-Galerkin (LSPG) PMOR method first presented in [1] was recently demonstrated in [2] for a challenging high-speed, turbulent, viscous flow problem past a complex fighter aircraft geometry. However, the state of the art of PMOR for CFD has been restricted to date to body-fitted meshes. The reason is that in general, embedded boundary models (EBMs) are not compatible with traditional PMOR frameworks due to their dynamic partitioning of the computational fluid domain into real and fictitious subdomains. Hence, complex flow problems that necessitate the use of an EBM for CFD–such as problems involving large shape changes, deformations, or topological changes–cannot be accelerated today by PMOR. Notable work pertaining to the initial development of a PMOR approach for EBMs includes the alternative right reduced-order basis (ROB) developed in [3], which accounts for the real/fictitious dynamic partitioning of the computational fluid domain. Here, this approach is generalized to more advanced EBMs than the standard ghost fluid method, which was the focus of the work in [3]. More importantly, it is equipped with hyperreduction–another challenging task to perform when the domain is dynamically partitioned into real and fictitious subdomains–to enable wall-clock time reduction. The result is a comprehensive framework for constructing nonlinear, projection-based reduced-order embedded boundary models for CFD and hyperreducing them using a variant of the energy-conserving sampling and weighting (ECSW) [4] method tailored for this purpose. This framework is demonstrated on a series of large-scale, convection-dominated CFD applications that necessitate the use of an EBM. It delivers significant wall-clock time speedup factors while maintaining accuracy.

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Reduced deep networks yielding stable nonlinear dimensionality reduction

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Key Words: Dimensionality Reduction, Deep Neural Networks, Nonlinear Model Reduction

There are inherent limitations to linear dimensionality reduction methods like the proper orthogonal decomposition (POD). To overcome these limitations, there has been recent interest in finding a nonlinear extension that retains many important properties of POD such as (1) the stability of the POD coefficients with respect to the data, or (2) the regularity in the POD modes. In this talk, we will discuss a generalization of POD to the nonlinear setting, in the form of a neural network called the reduced deep network (RDN) introduced in [1]. We present theoretical and numerical results showing that this extension yields a stable approximation to various datasets that proved challenging for POD in the past. We will focus on datasets taken from numerical solutions to nonlinear partial differential equations describing wave phenomena.

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Reduced Order Methods in Computational Fluid Dynamics: state of the art and perspectives

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Key Words: Model Order Reduction, Fluid Dynamics, Applied Sciences, Computational Science

We provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD). Efficient parametrisations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: a better use of stable high fidelity methods, considering also spectral element method and finite volume discretisations, to enhance the quality of the reduced model too, and allowing to incorporate some turbulent patterns and increasing the Reynolds number; more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; the improvements of the certification of accuracy based on residual based error bounds and of the stability factors, as well as the guarantee of the stability of the approximation with proper space enrichments. For nonlinear systems, also the investigation on bifurcations of parametric solutions are crucial and they may be obtained thanks to a reduced eigenvalue analysis of the linearised operator. All the previous aspects are very important in CFD problems to focus in real time on complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting with data assimilation or uncertainty quantification. Model flow problems will focus on few benchmarks, as well as on simple fluid-structure interaction problems and shape optimisation applied to industrial problems.

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Reduced Order Modeling for modular anisotropic Structures based on Proper Orthogonal Decomposition and Mesh Tying

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Key Words: Proper Orthogonal Decomposition, Mesh Tying, Anisotropy, Interpolation

A model order reduction technique in combination with mesh tying is used to efficiently simulate a large number of different structures that are assembled from a set of substructures. The stiffness matrices of the substructures are computed separately and assembled into a global stiffness matrix with tied contact formulation. The computational time can be further decreased by reducing the degrees of freedom of each substructure with a projection-based model order reduction technique. The precomputations to obtain the mode matrices are computationally cheap because they can be carried out on each substructure separately. For the development and optimization of new construction strategies for fiber reinforced concrete, a large number of different combinations of the modules have to be tested. The nonlinear anisotropic material behavior, like the primary directions of orthotropic materials [1], leads to parameter-dependent mode matrices. The precomputations can only be done for a relatively small number of parameters. For all other parameters, the mode matrices have to be adapted with interpolation methods to obtain an accurate solution [2].

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ROM Closures and Stabilizations for Under-Resolved Turbulent Flows

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Key Words: Reduced Order Models, Closures, Stabilizations, Data-Driven Modeling, Turbulent Flows

In this talk, I will survey reduced order model (ROM) closures and stabilizations [1] for under-resolved turbulent flows. Over the past decade, several closure and stabilization strategies have been developed to tackle the ROM inaccuracy in the convection-dominated, under-resolved regime, i.e., when the number of degrees of freedom is too small to capture the complex underlying dynamics. I will present regularized ROMs, which are stabilizations that employ spatial filtering to alleviate the spurious numerical oscillations generally produced by standard ROMs in the convection-dominated, under-resolved regime. I will also survey three classes of ROM closures, i.e., correction terms that increase the ROM accuracy: (i) functional closures, which are based on physical insight; (ii) structural closures, which are developed by using mathematical arguments; and (iii) data-driven closures, which leverage available data. Throughout my talk, I will highlight the impact made by data on classical numerical methods over the past decade. I will also emphasize the role played by physical constraints in data-driven modeling of ROM closures and stabilizations.

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A Computational Approach To The Effective Viscosity Of Non-Newtonian Fiber Suspensions

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Key Words: Fiber Reinforced Polymer, Fiber Suspension, FFT-based Computational Homogenization, non-Newtonian Fluid, Effective Viscosity

Due to their high specific stiffness and high degree of design freedom, fiber reinforced polymer components have been employed over a wide range of industries to facilitate technological progress. Manufacturing of fiber reinforced polymer components often involves fiber suspensions, for example the widely used injection and compression molding. Thus, an accurate understanding of the viscous properties of fiber suspensions is important for appropriate industrial application. Taking microstructural parameters into account, Fast Fourier Transform (FFT) based simulations enable high fidelity homogenization of mechanical properties of fiber suspensions [1].

Previous work [1] was restricted to FFT-based viscous homogenization under the assumption of a Newtonian polymer matrix. However, polymer melts usually show non-Newtonian behavior. Here we extend the computational methodology to shear thinning rheology by employing the Cross-WLF [2, 3] material model.

Based on a Newton method, we derive an efficient implementation of the cross fluid material model. We investigate the influence of microstructural parameters on the effective viscosity of fiber suspensions with a non-Newtonian matrix. We compare our results to effective viscosities of fiber suspensions with a Newtonian matrix and mean-field estimates. Finally, we identify sensitivities with respect to microstructural parameters.

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A Stable and Efficient finite element scheme for simulating Viscoelastic fluid flows

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Key Words: *Fractional Step method, Square Root transformation, Oldroyd-B*

This report presents an efficient stabilized finite element scheme for simulating viscoelastic flows at high Weissenberg numbers. The velocity and pressure variables in the momentum conservation equations are uncoupled using an incremental fractional step method based on the second order backward differentiation formula (BDF2). The pressure gradient projection (PGP) stabilization technique and the discrete elastic-viscous-split-stress (DEVSS) formulation are introduced into the scheme, in explicit versions, to circumvent the LBB constraints. For the constitutive equation, a square root transformation is firstly applied to retain the positive definiteness of the polymer conformation tensor, and then the streamline upwind/Petrov-Galerkin (SUPG) method and the second order Runge-Kutta scheme are employed for spatial and time discretizations. Three benchmark problems are tested and numerical results have revealed the accuracy and convergence of the scheme. What is more, since the presented scheme enables the use of equal low-order interpolations for all variables and requires no iterative process, it is computationally efficient and easy to be implemented.

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An adaptive rotated entropy stable scheme for the ideal MHD equation

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Key Words: Magnetohydrodynamics equation; Entropy stable scheme; Rotated angle; Adaptive moving grid; Runge-Kutta method.

The numerical solution of the magnetohydrodynamics(MHD) equation is of great significance in the fields of plasma physics, astrophysics research, and flow control. A rotated entropy stable scheme based on the moving grid is constructed for solving the ideal MHD equation. This method combines the Roe-type rotated entropy stable scheme based on the adaptive rotated angle and the adaptive moving grid algorithm, where the entropy stable scheme is used to discretize the MHD equation in space, and the grid evolution equation is constructed by the variational method and then is solved iteratively by Gauss-Seidel method for the adaptive grid. Furthermore, the method uses the conservative interpolation formula for the value transfer between on the new nodes and the old ones. And the rotated angle is defined by the velocity gradient function. The third-order strong stable Runge-Kutta method is used in time step. Numerical experiments show that the algorithm can effectively capture the structure of the solution (especially shock waves and rarefaction waves), and has high resolution, good versatility, and strong robustness.

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Efficient and Decoupled Schemes with Unconditional Energy Stability for the Block Copolymer Model in Copolymer/Homopolymer Mixtures

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Key Words: Block copolymer model, SAV approach, Step-by-step approach, Energy stability

In this talk, the numerical approximations of the Cahn-Hilliard type and conserved Allen-Cahn type block copolymer (BCP) model describing the phase separation of the copolymer and homopolymer mixtures are considered. We develop a series of efficient, unconditionally energy stable, non-iterative schemes based on the SAV, 3S-SAV, and new Lagrange multiplier approaches. The proposed numerical schemes lead to decoupled linear equations with constant coefficients at each time step, and their unconditional energy stabilities are proved rigorously. Numerical examples are provided to validate the accuracy and energy stability of the proposed schemes, and ample simulations are presented to show a variety of morphologies of pattern formations of the copolymer and homopolymer mixtures.

The finite element numerical investigation of gas entrapment phenomenon in non-isothermal polymer filling process

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Abstract: In this paper, the intricate gas entrapment phenomenon in the non-isothermal polymer filling process is investigated via a combined finite element and discontinuous Galerkin numerical algorithm. The evolving melt interface is captured via level set method and the eXtended Pom-Pom (XPP) constitutive model is employed to describe the viscoelastic fluid. The governing equations of flow field are solved via a coupled continuous and discontinuous Galerkin method. The implicit discontinuous Galerkin method is utilized for the solution of the XPP constitutive equation, level set and its re-initialization equations. The good agreement of experimental and simulation results illustrates the validity of this combined computational algorithm. The influence of injection velocity and the gate size on the gas entrapment phenomenon are both studied in the irregular cavity with complex insert. We have found that the entrapped gas is easy to appear for the case of higher injection velocity and smaller gate size. The distribution of temperature field in different cases are also shown.

Key Words: *gas entrapment, finite element; discontinuous Galerkin; XPP constitutive model, level set method*

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The SRCR-DG Method for Simulating Oldroyd-B Viscoelastic Fluid Flows

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Key Words: High Wi Number, Dual Splitting Scheme, High-Order Discontinuous Galerkin, Square-Root-Conformation

In this work, we present a high-order discontinuous Galerkin method (DGM) for simulating Oldroyd-B viscoelastic fluids at high Weissenberg (Wi) numbers. The dual splitting scheme is performed to decouple the velocity and pressure in the momentum and mass equations, and circumvent the limitation of the LB-B condition. The square-root-conformation representation (SRCR) method is applied in the constitutive equation to preserve the positive definiteness of the conformation tensor and improve the computational stability at high Wi numbers, and then the local Lax-Friedrichs flux and second-order Runge-Kutta scheme are employed for spatial and time discretization. Several typical benchmarks are considered to verify that the combinations of the dual splitting scheme, DGM and SRCR effectively improve the accuracy and stability compared with traditional methods for solving the Oldroyd-B viscoelastic flow problems at high Wi numbers.

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3D Transient Response of Layered Soils with Local Inhomogeneities

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Key Words: Soil Dynamics, Soil-Structure-Interaction (SSI), Integral-Transform-Method (ITM), Finite-Element-Method (FEM), Substructure technique, Elastic wave propagation

The three-dimensional dynamic interaction of surface foundations with structures buried in the ground or local geological inhomogeneities can have a significant impact on the structural responses and the wave propagation patterns in the ground. In particular, when amplification of ground motions occurs due to diffraction and scattering, it is essential to integrate these inclusions into prediction models and thus consider the Structure-Soil-Structure-Interaction (SSSI).

In this contribution an efficient 2.5D coupled Integral Transform Method (ITM) – Finite Element Method (FEM) approach [1] is used to compute the complex, dynamic stiffness at the surface of a layered soil including a longitudinally invariant structure or inhomogeneity. Herein, the analytical ITM solutions of the dynamic wave equation allow to account for the infinite extension of the soil by satisfying the radiation condition. The FEM enables to model complex, spatially limited structures and a part of the surrounding soil within a cylindrical outer boundary, on which both methods are coupled. The foundation on the ground surface is modelled using 3D finite elements and is coupled to the soil substructure enforcing the compatibility conditions at the common interface [2, 3].
By solving the overall system of equations in the frequency domain for an external load with unit amplitude over the entire frequency range, the transfer functions for the foundation compliances are calculated, weighted by the frequency spectrum of the transient load, and finally transformed to the time domain by an inverse Fourier transform.

The effect of soil stratification as well as embedment depth, size and stiffness of the inclusion on the transient foundation behaviour is investigated and interpreted by drawing correlations to the frequency spectra of the foundation compliances and power input at the soil-foundation interface. In addition, time-dependent displacement distributions on and within the soil are presented to illustrate the effects of the SSSI on wave propagation characteristics such as predominant wave types, propagation directivity, as well as interference and wave impeding effects due to the inclusion. For this purpose, a postprocessing procedure is used in which the interaction forces at the soil-foundation interface are applied as an external load to the soil substructure.

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Accuracy Analysis of Second-order-type Linear Multistep Time Integration Methods for Structural Dynamics

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Key Words: *Accuracy analysis, linear multistep methods, time integration, structural dynamics*

Abstract: The linear multistep (LMS) methods family had been a basic solving procedure for the ordinary differential equations, and also be a significant member of the time integration schemes for structural dynamics. They can be utilized solely for the equations of motion, such as the central difference method, the BDF2 method, the Houbolt method, etc; and can also be the sub-step methods of the composite schemes, such as the Park method, the Bathe methods family, etc. In addition, the accuracy analysis framework of the LMS methods had been extended to many single-step methods based on the spectral equivalence, such the Newmark-β method, the Wilson-θ method, the HHT-α method, the three-parameters optimal scheme, the GSSSS method, etc. The present study focuses on the second-order-type LMS methods which solve the second-order differential equations of motion directly. A generalized LMS methods family is considered, and a rigorous accuracy analysis is performed for desirable numerical properties. The accuracy conditions based on consistency, stability, convergence analyses are derived. Moreover, the error constant concept of the second-order-type LMS methods is developed. It has played an important role in the first-order-type LMS methods for algorithm optimization.

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An Energetic Boundary Element Method approach for Wavefield Modelling

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Key Words: Energetic Boundary Element Method, Time-Domain Wave Propagation, Infinite Media

Full-Waveform Inversion (FWI) is a challenging data-fitting procedure based on full-wavefield modeling to estimate the elastic parameters in the underground, in order to deduce a very detailed geophysical model. This can be achieved by minimizing the energy between the modeled and the field data using a gradient optimization approach. Key ingredients of the FWI are an efficient forward-modeling engine and a local differential approach, in which the gradient and the Hessian operators are efficiently estimated. In this light, the design of a suitable, efficient an accurate numerical method to solve the elastic forward problem is essential to develop a FWI strategy for an independent inversion of isotropic elastic material parameters. Even if different directions exist, the use of a Boundary Integral Equation (BIE) technique, whose discretization is known as the Boundary Element Method (BEM), is an appealing choice because it allows to handle problems defined on the exterior of bounded domains as easily as those defined in the interior, without the introduction of an artificial boundary to truncate the computational domain. Furthermore, this technique requires the discretization only of the domain boundaries, leading to a drastic reduction of the total number of degrees of freedom of the problem. Recently, a direct space-time Galerkin BEM for the discretization of time-domain BIEs related to 2D scalar and vector wave propagation problems has been introduced in [1] and [2]. This technique is based on a natural energy identity satisfied by the solution of the corresponding differential problem, which leads to a space-time weak formulation of the BIEs with precise continuity and coerciveness properties. Consequently, the integral problem can be discretized by unconditionally stable schemes with well-behaved stability constants even for large times. In this work, starting from optimal results obtained for 3D scalar wave propagation [3], we extend the energetic BEM to 3D realistic elastodynamic problems, showing the capabilities of the method of modelling a full wavefield rather than specific wave types.

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An improved Brownian dynamics for chromatin in human cells

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Key Words: *Brownian dynamics, collision, linker-DNA*

Eukaryotic chromatin chain with chromosomes is a physico-chemically stable material inside cell nucleus. Chromatin structure can be changed slowly or drastically through various physico-chemical interactions between nucleosomes, among which repulsion plays a key role in regulating material properties, genetic transcriptions, and gene expression. However, this type of physically driven changes is not fully understood, particularly in human cells. On the other hand, recent experiments in vivo reveals a dynamic liquid-like state of the polymer in a human cell [1]. This dynamic behavior has been observed in 100 milli second [2]. It suggests that the fluidity of the polymer and density effects of crowded molecules should be taken into account. And elastic response of linker-DNA is numerically estimated as non-linear. Therefore, it remains a crucial problem that Brownian dynamics simulation of the prototype Rouse model has a limitation of the short time step of 1ps to 1ns with the assumption of constant external force. Besides it is difficult to handle with the overstretching transition of a semiflexible polymer.

In this study, we aim to construct a simulation model of a chromatin fiber by improving Brownian dynamics with a time step longer than picoseconds, and by implementing the density effect of nucleosomal collisions. In our model, we proposed two plausible collision algorithms. One is to apply a wall solution to the Brownian process. As evaluation of the one, we confirmed diffusion property of nucleosomes which is similar to some estimated data. The other is to extrapolate the Brownian process from in-silico experiments of two-body collision. We treated nucleosomes as Brownian particles with Lenard-Jones interaction and spring interaction, and simulated the dynamics of these collisions in nanoseconds. Then, we constructed a probability function of a pair of nucleosomes based on the generalized collision process. As a result, we found that nucleosome displacements have characteristic distribution and we compared it with the wall solution algorithm. The results indicate that the Brownian collision process should be modified by our generalized extrapolated function.

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Application of the modified formal variational formulation to the Burgers' equation

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Key Words: Modified formal variational formulation, Conservation laws, Noether's theorem, Variational integrator

In the modelling and simulation of physical phenomena, numerical analysis of differential equations that represents the phenomena of objects can be evaluated based on stability, accuracy, and speed. In recent years, however, in addition to stability, structural conservation, i.e., whether the numerical method can reproduce the essential properties of the phenomenon, has been greatly emphasized. For variational systems, the symplectic structure is among one of the most important features, beside symmetries and conservation laws, which are connected by the celebrated Noether's theorem. One well-known efficient structure-preserving numerical methods for variational systems are variational integrators [1].

Unfortunately, many physical systems can not be naturally derived from variational calculus. The formal Lagrangian formulation was found useful for deriving conservation laws of some special non-variational systems [2] and for constructing their variational integrators [3]. This was extended to the modified formal variational formulation [4], which is applicable to arbitrary differential equations, that, on the one hand, allows us to derive conservation laws through Noether's theorem, and, on the other hand, provides necessary foundations for constructing variational integrators for arbitrary differential equations. In this talk, we will mainly be focused on applications of this novel method to the Burgers' equation.

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Filtering Spurious Eigenmodes in Electromagnetic Cavities Discretized by Energy-Orthogonal Twenty-Nodes Hexahedral Finite Elements

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Key Words: *Energy-Orthogonal Formulation, Electromagnetic Cavities, Spurious Eigenmodes*

An electromagnetic cavity as discussed in this contribution will be a source-free region enclosed by a perfect conductor and filled with a linear dielectric in which modes of free oscillation can exist at an infinite number of discrete frequencies. These standing-wave fields and natural frequencies are solutions of the eigenproblem associated with the double-curl operator. If the electric field is the variable solved then the magnetic field will be called the induced field, and vice versa. As is well known, if the operator double-curl is discretized with nodal finite elements then eigenspectrum computed will be severely polluted with spurious eigenmodes, the spurious eigenvalues having the same order of magnitude as the physical eigenvalues and not easily distinguished from them [1].

A standing-wave field can be represented by the superposition of plane harmonic waves travelling in several directions. For these fundamental wave solutions, by a dispersion analysis, the behavior of the energy density of the induced field is researched in unbounded domains discretized by regular meshes of twenty-nodes hexahedral finite elements formulated in energy-orthogonal form [2]. In this formulation the element stiffness matrix is split into basic and higher order components, which are respectively related to the mean and deviatoric components of the element induced field. This decomposition is applied to the element energy of the induced field and holds for the finite element assemblage. The first physical branch of the dispersion equations is selected for the analysis. The main results are summarized. Given the mesh, in the limit of long wavelength, although the energy density does not vanish, its higher order component does vanish. Similarly, given the wavelength, as the solution converges on account of mesh refinement, the energy density is increasingly dominated by its basic component. Nevertheless, the higher order energy density vanishes as a cancellation of the component associated with the vertex nodes and the one associated with the mid-side nodes, which do not vanish but are equal and opposite in sign. A sign characteristic is also satisfied by the vertex and mid-side components of the basic energy density. The convergence values of these energy components do not depend on the direction of wave propagation, direction of polarization, and mesh parameters. The relationship between the density of the mesh, the higher order energy density, and the energy error is researched for high precision discretization.

For cavities discretized by twenty-nodes hexahedral finite elements is proposed to accept only those eigenmodes for which the basic energy component of the induced field prevails over the higher order energy component. Additionally, the behavior of the vertex and mid-side energy components must be in accordance with the fundamental behavior deduced for these energy components by the dispersion analysis carried out for plane harmonic waves. The numerical research reveals that applying these energy constraints the spurious eigenmodes can be efficiently identified.

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Hybrid 3D-2D Finite Element Modeling for Elastodynamics

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Key Words: Coupling, Mixed-dimensional, Dimensional reduction, 3D-2D, 2D-3D, Panasenko, Hybrid model, Time-dependent, Elastic waves, Elastodynamics, Finite element.

Many engineering applications require the numerical solution of a large scale three dimensional (3D) or two-dimensional (2D) problem, which consists of a large number of degrees-of-freedom (DOF). Mixed-dimensional modeling suggests the reduction of a part of the domain in which the solution is expected to exhibit a lower-dimensional behavior to a domain of lower dimension, forming a hybrid multi-dimensional model with a significantly lower number of DOF. If designed properly, the hybrid model allows for reduced computational effort with small mixed-dimensional modeling error. Fields of application where mixed-dimensional modeling is of special interest include, among others, hydrological and geophysical flow models, blood-flow analysis, and elastic structures.

The coupling of 3D and 2D finite element (FE) models to form a single hybrid 3D-2D model is considered for linear elastodynamic problems. The research focuses on the way the 3D-2D coupling is performed, and on the coupling error generated. The Panasenko technique is used to couple the 3D and 2D models. This method has been used previously for mixed-dimensional coupling in steady-state problems [1], as well as for 2D-1D coupling of acoustic waves [2]. Here it is being used for the first time for the 3D-2D coupling of time-dependent elastic problems. The hybrid formulation is shown to be well-posed, and it is shown that the Panasenko method is extremely simple to implement in the framework of FE analysis, yet the resulting coupling yields a rather small error level, provided the 3D-2D interface is sensibly placed.

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Improvements in Semi-Implicit Integration Factor Method

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Key Words: Reaction-Diffusion, Matrix Exponential, IIF Method, Nonlinear solver, Parallelization

Stiff Reaction-Diffusion (R-D) equations are used to model various bio-chemical phenomena such as pattern formation and enzymatic reactions as well as motion of self-propelled particles [1].The stiffness of the problem necessitates the selection of very small time steps during numerical simulation of the equations if time-explicit integrators are used. The exponential integrator based methods such as implicit integration factor (IIF) [1] remove this constraint. Semi-implicit IIF has been used to model stiff R-D equations in several cases since it gives unconditional linear stability for second order accurate scheme [1]. This method, however, faces mainly two difficulties - computational efficiency of calculation of matrix exponential and time-complexity for nonlinear equations for large sized systems.

In this work, we address both the problems by proposing a novel method for calculation of matrix exponential and an algorithm for parallelizing the nonlinear solver. We calculate an approximation to the matrix exponential which reduces the computational time as well as memory usage during the computation of the exponential. For the nonlinear part we use GPU parallelization to improve the computational speed for 2D and 3D problems.

We simplify calculation of the matrix exponential by taking leverage of certain properties of the structure of the matrix exponential for 1-Dimensional Dirichlet problems. The matrix exponential of a large system is approximated using a smaller sized matrix without incurring significant errors. This leads to optimization of the memory usage of the matrix exponential as well as improvements in computational time compared to Padé approximation and scaling factor method used in MATLAB® *expm()* function.

The problem of time complexity of nonlinear solver is identified for R-D systems with the nonlinear reaction terms. The semi-implicit approach models the reaction term implicitly. This results in a nonlinear system which is decoupled from the evaluation of the linear diffusion term. We implement a parallelization algorithm to solve the nonlinear system. The presentation will first focus on the results of the matrix exponential approximation in comparison with MATLAB® *expm()* function. Secondly, we shall discuss the parallelization algorithm and its implementation for higher dimensional cases.

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Mixed Time Integrator for Finite Element Analysis of Wave Propergation in Nearly Incompressible Elasticity

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Key Words: Finite Element Method, Wave Propagation, Nearly Incompressible Elasticity, Mixed Time Integrator

In finite element procedures for dynamic problems of solid structures, explicit time integrators with relatively small phase error are suitable for calculating wave propagation phenomena[1]. However, they are conditionally stable and time increments should be determined from the propagation velocity of the elastic wave. When they are applied to nearly incompressible media such as rubber-like materials and biomaterials, very small time increments are required because of high velocities of P-wave representing volumetric deformations[2]. Therefore implicit time integrators with unconditional stability are usually adopted in such problems. In this work, a novel time integrator that posseses numerical properties of explicit time integrators in S-wave propegation is proposed[4]. To alleviates limitation of time increments, the present scheme is obtained by extending the Rattel method[3], which is proposed for constrained Hamiltonian systems.
In the proposed procedure, nearly incompressibility is considered using a u-p mixed finite element method with displacement and pressure as unknowns. An algorithmic relationship of volumetric strain with displacement and velocity is introduced to the Rattle method, in which constrained conditions must be treated implicitly. Further we derive an algorithm for solving linear equations with only pressure degrees of freedom, which is similar to the semi-implicit integrator by Kadapa[2]. The obtained method can be interpreted as a mixed time integration with an implicit solver for P-wave propagation and an explicit solver for S-wave propagation. Numerical experiments confirm that the numerical stability is determined by the Courant number of the S-wave. The mathematical analysis of the stability of the proposed method is also discussed.

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Numerical analyses on HELB-induced blast wave and jet impingement

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Key Words: *Blast wave, CEL analysis, jet impingement, structural integrity assessment*

A high energy line break(HELB) with operating conditions over 200 °F (93.3 ℃) or 275 psig (18.96 bar) involves physical phenomena such as pipe whip, jet impingement and blast wave that cause dynamic loads on structures, systems and components(SSCs) of nuclear power plants [1]. With regard to the HELB as a design basis event, a well-known design procedure [2] has been widely adopted. However, USNRC [3] recommended additional evaluation of amplificated blast wave through colliding with nearby SSCs and further conservative evaluation and realistic consideration of jet impingement. If HELB occurs, blast wave is first generated due to pressure difference between the compressed fluid in the line system and the air within a few milliseconds. Subsequently, jet impingement induced by the release of the fluid applies an irregular load on the SSCs. Since previous studies [4, 5] have been mainly conducted on independent phenomena, comprehensive researches to reflect these phenomena are needed for safe design.

The present study is to address blast wave and jet impingement evaluation under a typical HELB condition of 1,400MWe power plant. At first, dynamic load of blast wave was determined using computational fluid dynamics analysis, trinitrotoluene(TNT) equivalent approach and theoretical correlation. Coupled Eulerian-Lagrangian(CEL) analyses were also conducted to investigate structural effect of the load by applying a TNT explosive model. Then, dynamic characteristic model such as mode shape and effective mass ratio of the two component was made and power spectral densities(PSDs) were determined by using pressure-time histories from previous jet impingement assessment [5]. Based on the CEL analysis results, combined effect of blast wave and jet impingement were evaluated by performing random vibration analyses with PSD. Finally, structural integrity assessments of main components were carried out by comparing analysis results with allowable criteria for concrete and metallic materials.

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Numerical Simulation Of Ground Motion Field Effect Using Scaled Boundary Finite Element Method

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Key Words: *field effect, seismic wave propagation, overburden layer, fault fracture zone, topography*

Local site condition is an important factor affecting ground motion response , and it has a great influence on seismic wave field propagation and ground motion energy. Typical local site conditions, such as topography, layered site and fault fracture zone site, have always been a hot research topic. In this paper, the elastic wave equation is solved by using scaled boundary finite element method. The asymptotic transmission boundary is used to simulate the radiation of wave at the boundary towards half infinity. The ground motion response characteristics of these types of site models are studied, and the propagation characteristics of seismic wave field and amplitude characteristics of ground motion are calculated under the incident conditions of Rayleigh wave and SH wave. The effects of the order of interpolation function of the element, element size and integral method on the calculation results are discussed, and the results are compared with those of ABAQUS. The results show that the soft soli overburden layer site has amplification effect on the ground motion. The wave field conversion and coherence interaction on the interface of layered soil layer of the site lead to the amplification effect of the ground motion. The fault fracture zone in the fault fracture zone site has the effect of amplification and isolation on ground motion. When the seismic wave propagates to the fault fracture zone, it will reflect and refraction between the low-speed fault zone and the surrounding rock high-speed zone, and the wave field conversion and coherence will form the trapped wave. The local convex topography can amplify the seismic wave to some extent, but the seismic response of the local concave is small.

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Optimal Local Truncation Error Method for Solution of PDEs on Irregular Domains and Interfaces with Optimal Accuracy and Unfitted Cartesian Meshes.

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Key Words: *Numerical Method, PDEs, Optimal Accuracy, Unfitted Cartesian Meshes*

A new numerical approach called the optimal local truncation error method (OLTEM) is suggested for the solution of partial differential equations (e.g., see [1,2]). Similar to the finite difference method, the structure and the width of stencil equations are assumed in advance. Discrete equations include regular uniform stencils for internal points and non-uniform stencils for the points close to the boundary. The unknown coefficients of the discrete system are calculated by the minimization of the order of the local truncation error. The main advantages of OLTEM are an optimal high accuracy of discrete equations and the simplicity of the formation of a discrete (semi-discrete) system for irregular domains and interfaces (composite materials). For the regular uniform stencils without interfaces, the stencil coefficients can be found analytically. For non-uniform cut stencils, the stencil coefficients are numerically calculated by the solution of a small system of linear algebraic equations (20-100 algebraic equations). In contrast to finite elements, a trivial unfitted Cartesian mesh (no need in complicated mesh generators) is used with OLTEM. Changing the width of the stencil equations, different high-order numerical techniques can be developed. OLTEM does not include unknowns on irregular boundaries and interfaces. The known interface and boundary conditions at small number of selected points are added to the stencils as the right-hand side. Therefore, the width of 'boundary' and 'interface' stencils is smaller and equal to that for regular stencils. Currently OLTEM is applied to the solution of the wave, heat, Helmholtz, Poisson and elasticity equations. The theoretical and numerical results show that for the width of the stencil equations similar to that for linear finite elements, OLTEM yields the 4^{th} order of accuracy for the considered scalar PDEs on irregular domains (it is much more accurate compared with linear and high-order finite elements at the same number of degrees of freedom). E.g., 3-D numerical examples on irregular domains show that at accuracy of 5%, OLTEM reduces the number of degrees of freedom by a factor of greater than 1000 compared to that for linear finite elements with similar stencils. **At the computational costs of quadratic finite elements, OLTEM yields the 10^{th} order of accuracy for the time-independent elasticity equations and the 11^{th} order of accuracy for the Poisson equation with complex irregular interfaces.** This leads to a huge reduction in computation time for OLTEM at a given accuracy.

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Shape Identification of Scatterers Using a Time-Dependent Adjoint Method

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Key Words: *Adjoint method, Shape identification, Gradient, Inverse problem.*

This work deals with the inverse problem of *accurately* identifying the shape, size and location of scatterers in a 2D-membrane by measuring the signals of waves scattered from them. The proposed method is based on two stages. In the first stage we use the Arrival Time Imaging method [1] to significantly reduce the search area – there is no renewal in this stage. In the second and innovative stage, we load the membrane to generate waves which are being measured by a small number of sensors located at chosen points. Based on these measurements, an iterative process is performed to find the closed curve that represents the boundary of the scatterer. The process of translating the measured signals to a closed curve is an iterative process which minimizes a cost functional that represents the difference between the measured signals and the wave signals obtained in the presence of a candidate scatterer. The gradient of this functional, which represents its sensitivity to the scatterer geometry, is calculated efficiently using the adjoint method. Similar to what was done in [2], we discretize the unknown scatterer boundary from the outset, thereby allowing a simple and intuitive derivation of the adjoint formula for the gradient. The unknown curve is defined by a parametric representation that is completely general and does not make any preliminary assumptions about the scatterer geometry. A series of numerical example have been done, and showed that excellent identification is obtained even in the presence of noise, with a small number of sensors, and with no need for regularization. Additional different phenomena will be discussed during the lecture.

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Direct Method-based Gear Shakedown Analysis Considering Kinematic Hardening

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Key Words: *Gears, Shakedown Theorem, Tetrahedron Element Discretization*

In some working conditions, gears are subject to heavy-cyclic loads, such as wind turbines [1], and their failure modes are commonly caused by plasticity deformation accumulation. However, prior to the plasticity-induced failure, the shakedown states occurs when the increase of plastic strain ceases and the whole structure exhibits elastic response. Thus, the fatigue damages can be avoided by analyzing the shakedown loads of the gears in the plastic period.

Shakedown theory was first introduced in the 1930s, and Melan introduced the lower bound theorem that can be described: If the external cyclic loads vary within a scope, named *Load Domain L*, and a time independent self-equilibrium residual stress field $\overline{\boldsymbol{\rho}}$ of the structure body Ω and a load factor $\alpha > 1$ exists, shakedown happens in Ω under the defined *Load Domain L* when the superposition of $\overline{\boldsymbol{\rho}}$ and elastic stress arising from the external load. α is named as the shakedown factor, which determines the limit load of the shakedown state. Shakedown analysis has been widely utilized in fields of manned spacecraft, hull and pressure vessel. With respect to gears, Kapoor et al. [2] analyzed the shakedown limit of spur gears based on the upper and lower bound shakedown methods. He et al. [1] utilized the incremental method to evaluate the shakedown state of the two-dimensional turbine gear contact model considering the effects of residual stress and strain-hardening. However, it has the limitation of high computation costs and unsuitability in conditions that the loads' variation laws with time are unknown. In addition, due to the inadaptability of hexahedral element-based discretization on geometrically irregular gears, little research has focused on the shakedown limit of gears in a three-dimensional scale.

This abstract addresses these issues by proposing a shakedown theorem-based direct method for predicting the loading capacities of a typical industrial gear based on tetrahedral element-based discretization. For reducing the computation cost, the reduced Gaussian integration point scheme is applied to the elements to increase the efficiency of the computational algorithm. The rationality and precision of the proposed method are validated through a classical numerical model. The shakedown limit loads of the gear model under the perfect elastic-plastic and kinematic hardening material properties are compared, which demonstrates that the hardening material has a positive contribution to the loading capacity of the gear. It can be mainly explained by the witnessed redistribution of the residual stress field. The results demonstrate that the proposed direct method provides an effective means for predicting the limit loading capacity of gears under cyclic loading.

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15th World Congress on Computational Mechanics (WCCM XV)
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Hybrid High-Order methods for Electromagnetics

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Key Words: Polyhedral meshes, Hybrid High-Order method, Electromagnetics

Introduced in [2], the Hybrid High-Order (HHO) method provides a novel framework for the discretization of models based on PDEs. Its construction hinges on (hybrid) polynomial unknowns attached to both the cells and the faces of the mesh. HHO methods have several assets: (i) they are applicable on general polyhedral meshes, (ii) they allow for an arbitrarily large approximation order, and (iii) they are amenable to static condensation, thus allowing for a reduced computational burden.

The design of HHO methods for electromagnetics models is still in its infancy. As a matter of fact, there are (at least) three obstacles that make their devising highly challenging.

- The reconstruction of a local higher-degree potential (as standard in the HHO context) for the **curl** operator is nontrivial.
- The **grad**-**curl** orthogonality is lost at the discrete level.
- The well-posedness of the methods relies on (hybrid) discrete Weber inequalities [3], which are nontrivial to derive due to the fact that the HHO setting is non-compatible. The statement of the discrete Weber inequalities both strongly depends on the topology of the continuous problem, and on the choice of the discrete framework (discrete spaces and operators). Related discrete Maxwell compactness results are also nontrivial to prove.

This contribution will review the recent developments in the HHO approximation of (three-dimensional) electromagnetics problems [1]. This is a joint work with F. Chave and D. A. Di Pietro.

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Hybrid high-order methods for the fourth-order PDEs

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Key Words: Fourth-order PDEs, hybrid high-order method, stability, error analysis, computational performance, curved domains

We devise and analyze two hybrid high-order (HHO) methods for the numerical approximation of the Fourth-order PDEs problem. The methods support polyhedral meshes, rely on the primal formulation of the problem, and deliver $O(h^{k+1})$ H^2-error estimates when using polynomials of order $k \geq 0$ to approximate the normal derivative on the mesh (inter)faces. Both HHO methods hinge on a stabilization in the spirit of Lehrenfeld–Schöberl for second-order PDEs. The cell unknowns are polynomials of order $(k+2)$ that can be eliminated locally by means of static condensation. The face unknowns approximating the trace of the solution on the mesh (inter)faces are polynomials of order $(k+1)$ in the first HHO method which is valid in dimension two and uses an original stabilization involving the canonical hybrid finite element, and they are of order $(k+2)$ for the second HHO method which is valid in arbitrary dimension and uses only L^2-orthogonal projections in the stabilization. A comparative discussion with the weak Galerkin methods from the literature is provided, highlighting the close connections and the improvements proposed herein. Additionally, we show how the two HHO methods can be combined with a Nitsche-like boundary-penalty technique to weakly enforce the boundary conditions even on the curved domains. An originality in the devised Nitsche's technique is to avoid any penalty parameter that must be large enough. The numerical results showcase the efficiency of the proposed methods, and indicate that the HHO methods can generally outperform discontinuous Galerkin methods and even be competitive with C^0-interior penalty methods on triangular meshes.

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Virtual Element Method for Elliptic Hemivariational Inequalities arising in Contact Mechanics

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Key Words: Elliptic hemivariational inequality, Virtual element method, Contact mechanics

An abstract framework of the virtual element method is established for solving general elliptic hemivariational inequalities with or without constraint, and a unified a priori error analysis is given for both cases. Then, virtual element methods of arbitrary order are applied to solve three elliptic hemivariational inequalities arising in contact mechanics, and optimal order error estimates are shown with the linear virtual element solutions. Numerical simulation results are reported on several contact problems; in particular, the numerical convergence orders of the lowest order virtual element solutions are shown to be in good agreement with the theoretical predictions.

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Virtual element method for steady generalized membrane shell model

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Key Words: virtual element method, generalized membrane shell, polygonal mesh, cone shell, cylindrical shell

Virtual element method(VEM), a new numerical method with high regularity and flexible mesh, is being applied widely to Poisson problem, Stokes problem, linear elasticity problem, plate bending problem, biharmonic problem, Cahn-Hilliard problems, Steklov eigenvalue problem, some contact problems and so on. For two-dimensional shell models, this method has not been used. In this talk, we provide the VEM scheme for steady generalized membrane shell model for the first time. Concretely, conforming virtual element function space and degrees of freedom of the shape functions are proposed. A projection from the virtual element space to the polynomial space for this model is established. Then, the stability, convergence and error estimate of the discrete scheme are proven. Finally, we execute numerical examples involving a portion of a cone shell and cylindrical shell to verify the convergence and stability of the numerical scheme.

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A New TVD Scheme Based on BVD Principle

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Key Words: Finite Volume Method, Reconstruction, Total Variation Diminishing, Limiter Function, Boundary Variation Diminishing

The TVD (Total Variation Diminishing) scheme[1] is one of the high-order and numerically stable schemes for the finite volume method. The basic idea of this scheme is to suppress numerical oscillations by using the limiter function which satisfies the TVD condition. Although a variety of limiter functions have been proposed, it is hard to determine the optimal limiter for difference problems.

In addition, BVD (Boundary Variation Diminishing) schemes[2, 3] have been recently developed. This scheme effectively reduces the numerical dissipation error by following the BVD principle, which minimizes the jump of the left- and right-value of a reconstructed cell boundary value.

This study presents a new TVD framework based on the BVD principle. In the second order TVD region, the present scheme determines a suitable value of the TVD limiter function in the context of the BVD principle.

We compared numerical results using the present scheme with conventional TVD schemes in some benchmark tests for compressible flows. The present scheme is less dissipative near discontinuous solutions and capture small vortex structures caused by the Kelvin-Helmholtz instability. The new scheme also improves to avoid strange solutions due to the so-called squaring effect of some limiters. It is revealed that the combination of TVD and BVD frameworks has higher fidelity than the conventional TVD schemes.

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High-order low-dissipation TENO schemes: from structured to unstructured meshes

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Abstract: For compressible flow simulations involving both turbulence and shockwaves, the competing requirements render it challenging to develop high-order numerical methods capable of capturing the discontinuities sharply and resolving the turbulence with high spectral resolution. In particular, when deployed with the advanced large-eddy simulation (LES) approach, for which the governing equations are solved with coarse mesh, the solution is extraordinarily sensitive to the numerical dissipation resulting in large uncertainties for cross-code comparisons. In this talk, the family of high-order targeted essentially non-oscillatory (TENO) schemes are reviewed for general hyperbolic conservation laws with an emphasis on the high-speed turbulent flows. As a novel variant of the popular weighted ENO (WENO) scheme, the TENO scheme retains the sharp shock-capturing capability of WENO and is suitable for resolving turbulence with controllable low numerical dissipation. The key success of TENO relies on a strong scale-separation procedure and the tailored novel ENO-like stencil selection strategy. In addition, the built-in candidate stencils with incremental width facilitate the construction of arbitrarily high-order (both odd- and even- order) schemes featuring superior robustness. In this talk, the first-ever extension of TENO schemes to unstructured meshes with arbitrarily high-order reconstructions and mesh-element types will be presented. The tailored stencil arrangement and the new TENO weighting strategy for unstructured meshes will be elaborated. Detailed comparisons between WENO and TENO schemes with both structured and unstructured meshes will be discussed. Examples of the applications of TENO schemes to challenging compressible fluids with broadband length scales will be presented.

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Solution property preserving method for compressible turbulence simulation

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Key Words: *compressible turbulence, solution property preserving, BVD, MOOD*

The accurate simulation of complex flow including shock wave is a frontier and difficult problem in the field of computational fluid dynamics. Under the framework of finite difference and finite volume, researchers have developed a large number of classical shock capture methods. Although modern discontinuity-capturing methods have been able to solve the problem of shock capture, the methods still need to be further developed and improved for some complex flow phenomena including compressible turbulence simulation.

The solution property preserving method has been developed to simulate compressible turbulence, in particular, with strongly compressible characteristics. By combining the advantages of high-accuracy low dissipation scheme and high-resolution shock-capturing scheme, the method has obtained high-accuracy solution in smooth region and has suppressed numerical oscillation in discontinuous region. The method is implemented in the finite volume (FV) framework. Under the FV framework, based on the MOOD (multi-dimensional optimal order detection) concept, the hybrid computation of low dissipation reconstruction and solution property preserving reconstruction is realized, so as to give full play to the low dissipation characteristics of the central scheme and the shock capture ability of multi-step BVD (boundary variation dimensioning) scheme to the greatest extent.

Numerical experiments show that the developed method has good numerical characteristics such as low dissipation and positivity preservation, and can be applied to high accuracy simulation of compressible turbulence with and without wall bounded.

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Analysis and numerical simulations of viscoelastic phase separation

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Key Words: multiphase flows, viscoelastic flows, non-Newtonian fluids, relative energy, weak-strong uniqueness

We consider a viscoelastic phase separation model that describes phase-separation behaviour of a dynamically asymmetric mixture, which is composed of fast and slow components, see [1, 2].

In dynamically asymmetric mixtures the phase separation generally leads to the transient formation of network-like structures of a slow-component-rich phase and its volume shrinking. Consequently, in order to model such a rich dynamical behaviour the resulting viscoelastic phase separation model consists of the Cahn-Hilliard-type equation for two-phase flows and the Peterlin-Navier-Stokes equations for viscoelastic fluids. We will present our recent results on the global existence of weak solutions (also for degenerate mobility function) and the weak-strong uniqueness principle [3, 4, 5]. Numerical simulations are realized by an energy dissipative finite element method. Applying the relative energy we obtain the convergence of finite element solutions to a weak solution [6]. Numerical experiments will illustrate rich dynamical behaviour arising in the viscoelastic phase separation.

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Modelling and Simulation of Macroscopic Flows of Dense Suspensions

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Key Words: Suspension rheology, tensorial models, shear jamming, log-conformation tensor, finite element method, tensorial transport equations

The rheology of highly concentrated suspensions of solid particles dispersed in a viscous fluid features a number of surprising phenomena [1]. By varying the rate of deformation we can observe shear thinning, continuous or discontinuous shear thickening and, at very high concentrations, even the phenomenon of shear jamming. While the understanding of the microscopic origin of these phenomena has reached a significant depth [2, 3], the definition of suitable continuum-level models able to capture the rheology of dense suspensions is still the subject of active research efforts [4].

Building on a recently proposed tensorial model for shear-jamming suspensions [5], we develop constitutive relations that allow to include further effects such as shear thickening and yielding. In particular, the inclusion of rate-dependent phenomena requires the addition of evolution equations for tensorial measures of strain, akin to the conformation tensors used in viscoelastic fluid models. The presence of such evolution equations and the nonlinearities that arise in coupling them to the flow equation require appropriate computational strategies to guarantee the reliability of the numerical results [6].

Different features of the proposed continuum model are analyzed and illustrated with numerical solutions in paradigmatic examples of complex flows, in which the geometric features of the domain and the possible presence of free surfaces make it necessary to have available a fully tensorial model. In parallel, we discuss the numerical strategies employed to treat such heterogeneous flows.

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Numerical investigation of binary collisions of non-Newtonian droplets

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Key Words: *Numerical solution, droplet collision, viscoelastic fluids, Front-tracking*

We have numerically investigated the binary collision of viscoelastic drops by using a Front-tracking/Marker-And-Cell methodology. The numerical scheme is validated with shear-thinning fluids under surface tension effects. After, we have solved the droplet-droplet dynamics for viscoelastic constitutive models of Oldroyd-B and Phan-Thien-Tanner (PTT). In order to describe our main finding, maps of outcomes as functions of the dimensionless numbers that govern the problem are provided.

The simulations describe the bouncing, coalescence, and separation outcomes varying the Weber number as well as Weissenberg number. Our findings suggest that surface tension and elasticity act to maintain the integrity of the merged drop and avoid separation.

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Second-order finite difference approximations of the upper-convected time derivative

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Key Words: Generalized Lie derivative, Lagrangian scheme, Finite difference method

For $d \in \{1,2,3\}$, the velocity $u : \Omega \times (0,T) \to \mathbb{R}^d$ and a tensor $\zeta : \Omega \times (0,T) \to \mathbb{R}^{d\times d}_{\mathrm{sym}}$ to represent the non-Newtonian contribution, we focus on the so-called upper-convected time derivative or Oldroyd derivative $\overset{\triangledown}{\zeta}$ defined by $\overset{\triangledown}{\zeta} := \partial\zeta/\partial t + (u\cdot\nabla)\zeta - (\nabla u)\zeta - \zeta(\nabla u)^\top$, which usually appears in the constitutive equation of popular viscoelastic models, cf., e.g., [1]. It is worthy to note that the idea of the generalized Lie derivative can reformulate the upper-convected time derivative, cf., e.g., [2]. In this talk, based on [3], we firstly present a two-step second-order approximation in time for $\overset{\triangledown}{\zeta}$. Secondly, we propose new finite difference approximations for the upper-convected time derivative. The theoretical analysis of the truncation errors of the finite difference approximations considers the linear and quadratic interpolation operators with a Lagrangian framework. Thirdly, we present numerical results illustrating the theoretical results for a model equation for $d = 1$ and 2. Finally, we also apply the finite difference approximations of second-order in time for solving a two-dimensional Oldroyd-B constitutive equation subjected to a prescribed velocity field at different Weissenberg numbers.

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Development of structural analysis code based on FEM for aircraft design simulator using CFRP and CFRPT

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Key Words: *FEM, Shell and beam, Inertia relief, Geometrically nonlinear, Superelement*

In the New Energy and Industrial Technology Development Organization (NEDO) project "Toward Ideal Aircraft-Structure Design with Carbon Fiber Reinforced Thermoplastics", structural analysis code has been developed based on the finite element method. This code is referred to as *NLFEASTR*, and used for aircraft design simulations using carbon-fiber-reinforced plastics and thermoplastics (CFRP and CFRPT). The code uses structural elements including shell elements such as MITC4 [1] and MITC3 [2] and beam elements, and can perform static analyses, eigenvalue analyses for natural frequency and buckling load, and transient analyses. In addition, it has the following capabilities.

- An inertia relief function to perform static analysis for unconstrained structures subjected to a constant external load
- A geometrically nonlinear analysis function to consider large deformations and rotations of a structure
- A superelement technique to reduce the size of the finite element model
- A shear panel element for buckling tolerance design analysis

In the presentation, an outline of the developed code *NLFEASTR* will be given, and numerical results that verify its functions will be provided.

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High-Fidelity Wall-Modeled LES around Full Aircraft Configuration near Stall Condition

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Key Words: CFD, wall-modeled LES, full aircraft configuration, hierarchical Cartesian, KEEP scheme

This study presents the wall-modeled LES of complex flows around full aircraft configuration at stall condition using hierarchical Cartesian meshes. The key numerical methods in the presented wall-modeled LES are the wall-modeling on non-conforming wall boundaries [1], the non-dissipative kinetic energy and entropy preserving (KEEP) scheme [2], and the conservative low-pass filter on the hierarchical Cartesian mesh[3], proposed in our group. The aircraft configuration is the JAXA standard model (JSM) which involves high-lift devices. The presented wall-modeled LES successfully predicts lift coefficient, pressure distribution, and flow separation (Fig. 1). Additionally, compared to the conventional upwind scheme, the advantages of the non-dissipative nature of the KEEP scheme are demonstrated (Fig. 2).

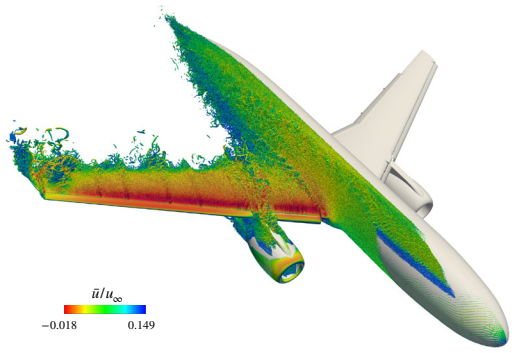

Figure 1: Instantaneous iso-surfaces of Q criterion.

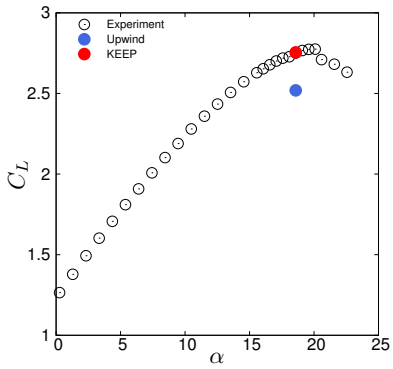

Figure 2: Lift coefficient C_L.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Integrated Analysis of Operating Engine and Airframe for High-Fidelity Wing Load Estimation

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Key Words: CFD, High-Fidelity Aerodynamic Evaluation, Operating Engine, Airframe

This study integrated and analyzed an operating engine with an airframe. The engine simulates 22 rotors and a passage on NASA Rotor 67; the airframe consists of a fuselage, a wing, a nacelle, and a pylon based on NASA Common Research Model. In the past developments, engines were designed alone; they modeled the intake flow distribution affected by the airframe. For the high bypass ratio engines expected to be developed in the future, it is desirable to estimate the engine's performance in a form faithful to the practical engine without modeling because past knowledge is insufficient. This study would enable us to assess the high-fidelity aerodynamic loads on the main wing and accomplish an ideal structural design. The engine and fuselage are discretized separately and analyzed in an integrated manner using the overset mesh method, and the flow at the engine inlet is estimated without modeling. An unstructured mesh method, suitable for designing complex 3D geometries of engines and airframes, is adopted to ensure robustness to their changes. Since the analysis was successfully running, we would examine the mesh dependency and verify the validity of the results by comparing them with experimental data.

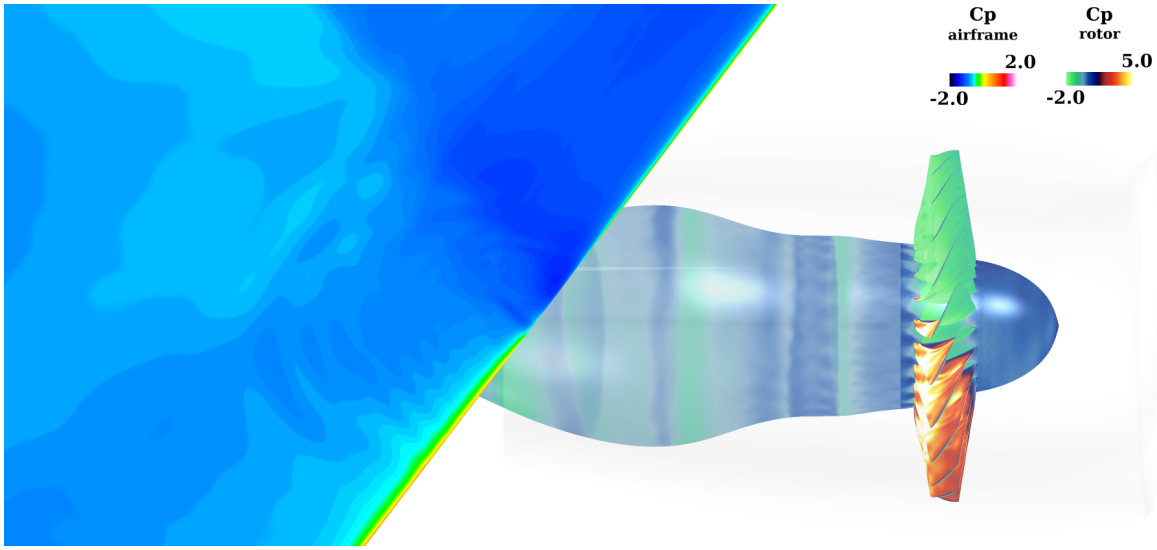

Figure 1: C_p distributions on the rotor, the passage, and the wing upper surface at rotating four-pitch (4/22). We look down on the computational object from above; the nacelle and the pylon are depicted in translucent view.

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Muti-objective design exploration approach for aircraft wing design with carbon fiber reinforced plastics

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Key Words: Aircraft Design, Fluid-Structure Interaction, Optimization, CFRP

Digital design of aircraft has been one of the most challenging topics in engineering fields, which requires highly multidisciplinary simulation tools and has yet to be fully realized in industries [1]. This study has developed a multiscale design framework of aircraft wings with carbon fiber reinforced plastics (CFRPs), wherein a multiobjective design exploration of wing geometries has been performed using a genetic algorithm [2]. Figure 1 represents a preliminary optimization results for different carbon fibers, i.e., T800S (black) and T1100G (red), where two objective functions are adopted: minimization of the drag and structural weight under the constraint of a specified lift coefficient ($C_L = 0.5$). The plot shows a reasonable result that the stiffer fiber leads to a lighter weight.

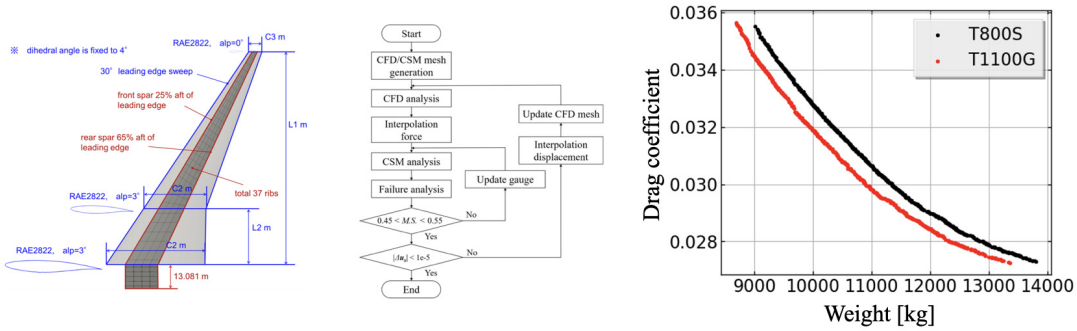

Figure 1: Multi-objective design exploration of CFRP wings

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New calculation scheme for compressible Euler equation

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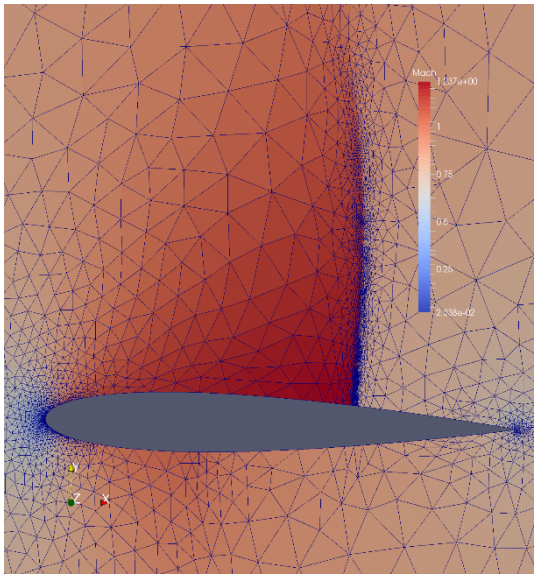
Key Words: *Compressible Euler equation, Finite element method, NACA0012*

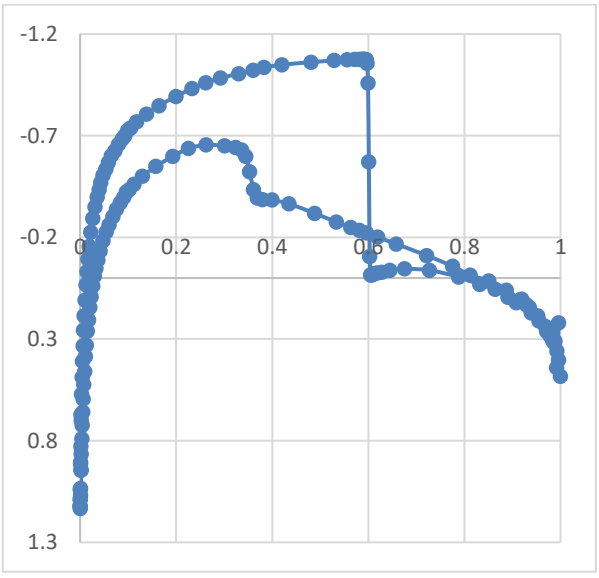
F. De Vuyst (HAL Id : cel-00842234, ver. 1) suggests a new mathematical model for compressible Euler equation as follows;

$$\frac{Da_\rho}{Dt} + \nabla \cdot \boldsymbol{u} = 0, a_\rho = \log(\rho),$$
$$\frac{1}{T}\frac{D\boldsymbol{u}}{Dt} + \nabla a_p = 0,$$
$$\frac{Da_p}{Dt} + \gamma \nabla \cdot \boldsymbol{u} = 0, a_p = \log(p).$$

In general, compressible fluid is calculated by using finite volume method (FVM) or discontinuous Gelerkin method (DGM), to gurantee high numerical calculation accuracy. However, these discritizing sheme is needed high calculation cost. The above mathematical model is able to be used standard Gelerkin method with lower calculation cost than FVM and DGM. In this presentation, NACA0012 is adopted as a first trial domain, and calculation results are very similar to previous results.



(a) Mach number and FEM mesh.



(b) Pressure distribution on NACA0012.

Figure 1. Numerical simulation results.

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A nonlinear elimination preconditioned inexact Newton method for blood flow problems in human artery with stenosis

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Key Words: Blood flow problem, inexact Newton method, nonlinear preconditioning, parallel computing

Simulation of blood flows in the human artery has become a powerful tool for understanding the hemodynamics. The blood flow is often smooth in a healthy artery, but may become locally chaotic in a diseased artery with stenosis, and as a result, a traditional solver may take many iterations to converge or does not converge at all. To overcome the problem, we develop a class of nonlinear preconditioning algorithms in which the variables associated with the stenosis are iteratively eliminated and then a global Newton method is applied to the smooth part of the system. More specifically, we model the blood flow in a patient-specific artery based on the unsteady incompressible Navier-Stokes equations with resistive boundary conditions discretized by a fully implicit finite element method. The resulting nonlinear system at each time step is solved by using an inexact Newton method with a domain decomposition based Jacobian solver. To improve the convergence and robustness of the Newton method for arteries with stenosis, we develop an adaptive nonlinear elimination preconditioner which performs subspace correction to remove the local high nonlinearities. Numerical experiments for several cerebral arteries are presented to demonstrate the superiority of the proposed algorithm over the classical method with respect to a variety of physical and numerical parameters. We also report the parallel scalability of the proposed algorithm on a supercomputer with thousands of processor cores.

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Classification of in Vivo Mice Magnetic Resonance Imaging for Early Detection of Liver Fibrosis by Machine Learning Technique

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Key Words: MRI segmented, Noninvasive, Liver fibrosis, Support Vector Machine (SVM)

In recent years, chronic liver disease has been a severe disease that affects health, and in the early stage of liver fibrosis, there are possible ways to restore health through treatment and diet. At present, noninvasive diagnosis methods such as blood tests and abdominal ultrasound are not easy to detect the early stage of liver fibrosis. In this work, we proposed using a machine-learning (ML) technique to predict the stages of liver fibrosis, classified as healthy, mild, or severe, through mice in vivo experiments. Specifically, we employed a support vector machine as the classifier. Two types of features, namely the simply connected domain scores and estimated porosity related to liver fibrosis from mice's magnetic resonance (MR) imaging, are used to train the classifier. The basic idea of these two feature extractions is originated from the geometric and topological properties of liver imaging. After parameter tunning, the classification accuracy of our proposed method for the testing result outperformed a baseline, convolution neural network method (CNN), 95.5% versus 87.8%. We demonstrated that the ML method, in conjunction with suitable features extracted from MR images, can be served as a diagnostic tool for the stage of liver fibrosis.

Computational Fluid Dynamics in Intracranial Atherosclerotic Disease: The Clinical Implications

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Background and objectives: Intracranial atherosclerotic disease (ICAD) is an important cause of stroke, particularly in East Asian populations. Those with an ischemic stroke attributed to ICAD (i.e., symptomatic ICAD) face a considerable risk of stroke relapse despite contemporarily best medical treatment. We aimed to investigate the clinical relevance of cerebral hemodynamics in symptomatic ICAD, assessed via a computational fluid dynamics (CFD) model.

Methods: In a series of studies, we used a CFD model constructed based on computed tomography angiography images to simulate blood flow across the symptomatic ICAD lesion, in patients with an ischemic stroke or transient ischemic attack attributed to ICAD with 50-99% luminal stenosis. Translesional pressure ratio (PR) and translesional wall shear stress ratio (WSSR) were obtained in the CFD model to quantify the relative changes of these two hemodynamic metrics across a symptomatic ICAD lesion, when a low PR (relatively large pressure gradient across the lesion) and high WSSR (significantly elevated wall shear stress upon the lesion) indicate a hemodynamically more severe ICAD lesion.

Results: We found that symptomatic ICAD patients with a low PR and a high WSSR had a significantly higher risk of recurrent ischemic stroke in the same territory than those with normal PR and WSSR, despite best medical treatment, with hypoperfusion and/or artery-to-artery embolism as the probable mechanisms of most of the recurrent strokes. We have also identified a significant association between wall shear stress measures across symptomatic ICAD lesion and progression/regression of luminal stenosis in the lesion in medically treated patients. Moreover, we have associated low PR and high WSSR with more severe covert cerebral small vessel disease burden in the ipsilateral hemisphere, in those with symptomatic ICAD in the anterior circulation.

Conclusions: Cerebral hemodynamics plays an important role in governing lesion evolution and the mechanisms and risk of stroke in ICAD, which may also underlie the development/progression of cerebral small vessel disease. There could be wide applications of CFD models in investigating the clinical implications of cerebral hemodynamics in ICAD and other cerebrovascular diseases.

High Resolution Patient-specific Blood Flow Simulations with High Performance Computing

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Key Words: *Blood Flow Simulations, Parallel Computing, Domain Decomposition Method*

Patient-specific blood flow simulations have the potential to provide quantitative predictive tools for virtual surgery, treatment planning, and risk stratification. To accurately resolve the blood flows based on the patient-specific geometry and parameters is still a big challenge because of the complex geometry and the turbulence, and it is also important to obtain the results in a short amount of computing time so that the simulation can be used in surgery planning. In this talk, we will discuss some scalable parallel methods for the simulation of blood flow in compliant arteries on large scale supercomputers. The blood flow is modelled by 3D unsteady incompressible Navier-Stokes equations with a lumped parameter boundary condition, which are discretized with a stabilized finite element based on unstructured meshes in space and a fully implicit method in time. The large scale discretized nonlinear systems are solved by a parallel Newton-Krylov method preconditioned by linear and nonlinear domain decomposition preconditioners. Some patient-specific cases with clinical measured data are used to verify the accuracy of the simulation results and show the performance of the algorithms. Numerical results show that the proposed methods work well for realistic geometry and parameters on a supercomputer with thousands of processor cores. A patient-specific analysis, with a resolution higher than 4D MRI can be obtained in less than one hour.

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The Effective Stiffness of 3-Dimensional Heterogenous Structures Derived by 1-Dimensional Finite Element Meshes

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Key Words: Effective Stiffness, 3D Graph, Finite Element, FEA, Porous, Heterogenous

Applications with anisotropic structures require a precise description of their mechanical properties. While recurring shapes are accessible for detailed investigations by homogenization methodologies, naturally grown, heterogenous structures like the human bone tissue with no identifiable unit cell need a different approach for material characterization. Rietbergen et al. demonstrated the computation of such information by direct numerical simulation [1].

In this Publication, we propose the modeling of porous, heterogenous and anisotropic structures, by their transformation into an equivalent 3D graph. The graph is retrieved by thinning the plates and struts of the structures into lines of a discrete width of one voxel. In a subsequent step, the irregular lines are converted into straight lines, defined by the position of their adjacent nodes.

By directly discretizing the graph with 1D elements like beams or trusses, a mesh of finite elements is created. The total mesh gets decomposed by intersection with control volumes of a user defined size and shape. The effective stiffness matrices of the control volumes are derived by numerical evaluation of their finite element structure according to Schmid [2].

In principle, the computational effort of the proposed methodology depends on the algorithms to transform the image into a 3D graph, the density of the anisotropic structure and the type of 1D finite elements, used to discretize the graph. Additionally, the order of the macroscopic elements representing the control volumes for which the effective stiffnesses are calculated has an impact on the performance of our method.

We will show, that our methodology, due to the 1D FEA approach, requires lower computational effort compared to the methodology proposed in [1], while preserving an accurate mechanical representation.

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A Matrix–Free Approach for Smoothed Aggregation Algebraic Multigrid

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Key Words: Multigrid, Algebraic Multigrid, Matrix-Free, GPU

In the past decades, the advancement of software and algorithms has allowed multigrid (MG) algorithms to take advantage of the computational benefits provided by graphics processing units (GPUs) in more advanced machines. These MG solvers are often referred to as geometric MG (GMG) or algebraic MG (AMG) based on whether transfers between grids are constructed using geometric or algebraic properties of the problem being solved. The main difficulties of working with GPUs are latency of memory transfers and lower memory storage abilities, meaning many traditional algorithms require changes in order to utilize the acceleration provided by GPUs to the fullest extent. Recently, GMG frameworks have been introduced for matrix–free (MF) finite element methods (FEMs) [1], where the matrix resulting from the FEM discretization is never stored explicitly, but instructions for application of the matrix as an operator are stored instead and utilized in the MG hierarchy. This approach greatly reduces the memory footprint of the algorithm and takes advantage of GPUs better than traditional solvers for FEMs. However, due to the nature of many AMG algorithms querying individual values of a matrix to construct grid transfers, MF AMG solvers are not commonly explored.

We present a matrix–free approach for smoothed–aggregation (SA) based AMG [2] for FEMs. Our approach constructs the FEM operator for the matrix via sum factorization and constructs the AMG coarsening operators by querying the matrix operator through its application against carefully chosen inputs without explicitly storing the fine matrix in memory, leading to performance benefits for the algorithm on GPUs. We discuss the algorithm and then present its implementation in the MueLu MG library, and we present results including scaling studies, comparisons with existing SA–AMG approaches within MueLu, and comparisons with MF approaches in other scientific software libraries. Finally, we discuss the impact of this work within the context of MFMG solvers for FEMs and directions for future work.

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A scalable and robust *p*-multigrid preconditioner with a vertex-star relaxation for high-order FEM

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Key Words: Preconditioning, High-order, Tensor product, Additive Schwarz, Sparse Cholesky

Pavarino [1] proved that the additive Schwarz method with vertex patches and a low-order coarse space gives a *p*-robust solver for symmetric and coercive problems. However, for very high polynomial degree it is not feasible to assemble or factorize the matrices for each patch. In this work we introduce a direct solver for separable patch problems that scales to very high polynomial degree on tensor product cells. The solver constructs a tensor product basis that diagonalizes the blocks in the stiffness matrix for the internal degrees of freedom of each individual cell. As a result, the non-zero structure of the cell matrices is that of the graph connecting internal degrees of freedom to their projection onto the facets. In the new basis, the patch problem is as sparse as a low-order finite difference discretization, while having a sparser Cholesky factorization. We can thus afford to assemble and factorize the matrices for the vertex-patch problems, even for very high polynomial degree. In the non-separable case, the method can be applied as a preconditioner by approximating the problem with a separable surrogate. We apply this approach to high-order discretizations of incompressible neo-Hookean hyperelasticity.

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Analysis of multigrid methods for systems of PDEs using structured matrices

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Key Words: Multigrid methods, systems of PDEs, structured matrices

Systems of partial differential equations are of interest in many applications in engineering, e.g., the elasticity equations or the Stokes equations. For large-scale simulations multigrid methods are often the method of choice, as they provide an efficient way of solving the associated linear systems. In the case of geometric multigrid methods the analysis is usually carried out using Fourier analysis. This does not allow for an asymptotic multilevel analysis and becomes relatively complicated for systems.

Instead, we use structured matrices, i.e., Toeplitz matrices or circulant matrices, and traditional multilevel theory to analyze the properties of the multigrid methods. While this approach is similar to Fourier analysis, an estimate of the convergence rate is also possible for the multilevel case. For scalar problems, including those arising from the discretization of PDEs, this technique has been studied intensively. Recently, we started transfering these results to the systems case that results in block-Toeplitz matrices or block-circulant matrices [1]. Besides studying higher-order discretizations of scalar PDEs, systems of PDEs also fit in this framework.

The usage of structured matrices allows for a rigorous treatment of different discretizations (finite differences, finite elements, finite volumes) and the analyses carry over to non-constant coefficients and more complex triangulations. Further, the multilevel hierarchy arises naturally and the multiplication with structured matrices and multgrid methods for them can be implemented on modern computer architectures in a very efficient manner.

In the talk the analysis technique, the derived sufficient conditions for optimal convergence and numerical results will be presented. Further, the application to problems in mechanics will be discussed.

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Block smoothers within geometric multigrid methods for the solution of the Stokes equations

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Key Words: numerical mathematics, geometric multigrid methods, Stokes equations, block smoother, local Fourier analysis, finite difference discretization

Multigrid (MG) methods are efficient methods to solve systems of partial differential equations (PDEs). They are used to speed up linear system solves in a wide variety of applications. The efficiency of multigrid methods is due to the combination of suitable smoothers with a coarse grid correction. As one of the two key ingredients, smoothers have a significant impact on the performance of multigrid solvers. Most of the literature on smoothers in multigrid methods is concerned with scalar PDEs, only. Systems are considered less often. This talk is concentrated on the development and analysis of new smoothers within geometric multigrid methods for the solution of the Stokes equations discretized on staggered grids. We compare the commonly used Vanka smoother with a non-overlapping variant of the Vanka smoother, the so-called triad-wise smoother. While the latter is computationally cheaper, the convergence depends much more on the implementation than that of the overlapping method. We develop new non-overlapping smoothers, the so-called fourfold triad-wise smoothers, and show their efficiency within multigrid methods to solve the Stokes equations. Local Fourier analysis and a general comparison including the computational cost and the convergence properties of the overlapping and non-overlapping methods will be presented.

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Multilevel Methods for Constrained and Non-linear System

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Key Words: Contact and fracture problems, multiphysics Problems, non-standard discretization, non-linear problems

Multilevel methods are well established for the solution of sparse linear systems. For constrained and non-linear systems, however, multilevel methods need to be adapted in order to ensure multilevel efficiency as well as global convergence. In this talk, we will provide an overview on multilevel approaches for constrained and non-linear systems and will provide several examples for problem dependent multilevel decompositions.

As examples, we will present multilevel solution strategies for constrained and non-linear systems, as they arise in the simulation of, e.g., contact problems or coupled non-linear problems in mechanics. We will start our discussion with the designing multilevel decompositions for contact problems in linear elasticity, i.e., convex minimization problems with inequality constraints, and will investigate how these multilevel decompositions do depend on the respective discretization. Starting from classical primal discretizations, we will consider the case of mixed finite elements in the context of least square finite element methods and eventually non-fitting discretization techniques. We will show how efficient multilevel methods for these different discretizations can be developed and which particularities have to be taken into account. We then will comment shortly on the case of non-linear problems, which here will be phase-field problems for fracture propagation. We will derive efficient multilevel decompositions for this problem class and will discuss the design of multilevel decompositions for non-linear problems. For all cases we will discuss the convergence properties of the resulting non-linear or non-smooth multilevel methods. Our findings will be illustrated by different numerical examples.

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Non-invasive Regional Multigrid for Semi-structured Grids

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Key Words: Multigrid Methods, Geometric Multigrid, Algebraic Multigrid

In this talk we discuss the development of a framework for multigrid solvers targeted at semi-structured meshes. In terms of exascale computing, memory, and setup time, there are significant potential advantages to multigrid on structured meshes over unstructured meshes. Unfortunately, many applications are not conducive to the use of structured meshes. Thus we focus on semi-structured meshes which provide flexibility to address complex computational domains while still allowing most multigrid calculations to be accomplished using efficient structured grid ideas and kernels. These semi-structured meshes center around the concept of block structured or region structured grids, and are created from the union of of a number of fully structured meshes that are each prescribed on subdomains and that conform at region interfaces. The idea behind these meshes can be further relaxed to allow for some unstructured mesh regions when needed.

We present a formal mathematical framework for describing the semi-structured solver. This formalism allows us to precisely define the associated regional multigrid method and to show its relationship to a more traditional multigrid solver. Additionally, the mathematical framework clarifies the associated software design and implementation. Numerical experiments highlight the relationship of the new solver with classical multigrid. We also demonstrate the generality and potential performance gains associated with this type of semi-structured multigrid as well as showcase its application to meshes with structured/unstructured mesh interfaces.

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Physics-based block preconditioning for beam/solid interaction

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Key Words: Physics-Based Block Preconditioning, Algebraic Multigrid, Sparse Approximate Inverse

Algebraic multigrid (AMG) methods have shown to be highly efficient and scalable preconditioners for mortar methods ranging from contact to meshtying problems [1]. An interesting application in this field is the mixed-dimensional coupling of slender beam structures embedded into three-dimensional solid bodies [2]. Such beam/solid interactions can be found in several engineering scenarios (e.g. fiber-reinforced composite materials or reinforced concrete). Imposing the coupling constraints via a penalty method as proposed in [2] leads to an ill-conditioned and highly non-diagonal dominant matrix. Solving such problems in an efficient and scalable manner with iterative solvers is difficult and makes an appropriate preconditioning essential. Using AMG in this context is yet again challenging as there are several open questions regarding AMG for beams and the coarsening of the mixed-dimensional coupling terms.

This talk will discuss a physics-based block preconditioning approach based on AMG. The outer block iteration is taken care of with an inexact LU-decomposition. A crucial part of the calculation is the approximation of the inverse appearing in the Schur complement. Using a sparse approximate inverse [3] based on an appropriate sparsity pattern helps to retain a low iteration number and parallel scalability. Multilevel ideas will be used to approximate the block inverses appearing in the system. There, the computation of the near nullspace of the beam part is highlighted, which effectively projects the errors onto a coarser grid. We will assess the performance of the proposed block preconditioner using examples of the interaction of solids with torsion-free Kirchhoff-Love beam finite elements.

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Three-level Overlapping Schwarz Methods on the Theta Supercomputer

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Key Words: Domain Decomposition, Fast and Robust Overlapping Schwarz (FROSch), High Performance Computing, Many-Core, Trilinos Software Library

A new approach to three-level overlapping Schwarz domain decomposition methods of GDSW (Generalized Dryja-Smith-Widlund) type for linear elasticity is presented. This approach was recently implemented in the Fast and Robust Overlapping Schwarz (FROSch) framework [1, 2], which is part of the Trilinos software library [3]. In this approach, no explicit geometric information is needed in the recursive application of the preconditioner.

Parallel results for a three-dimensional linear elasticity problem obtained on the Theta supercomputer (ALCF, Argonne, USA) using up to 220 000 cores are discussed and compared to results previously obtained on the SuperMUC-NG supercomputer (LRZ, Garching, Germany).

Notably, it can be observed that a hierarchical communication operation in FROSch related to the coarse operator starts to dominate the computing time on Theta for 100 000 MPI ranks or more. The same operation, however, scales well and stays within the order of a second in all experiments performed on SuperMUC-NG. Using hybrid MPI/OpenMP parallelization, better performance is achieved on Theta.

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A Robust Tree-matching Algorithm for Diagnosis of Bronchiectasis

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Key Words: *Interstitial pneumonia, Bronchiectasis, Graph theory, Tree-matching*

The target of this research is efficient assessment for interstitial pneumonia. Interstitial pneumonia shows several imaging findings on computed tomography, among which traction bronchiectasis/bronchiolectasis is useful to predict disease progression. This imaging finding is represented by irregular bronchial and bronchiolar dilatation, which are caused by retractile pulmonary fibrosis affecting the surrounding tissues. When a physician assesses a patient, whether the patient's condition is getting better or getting worse, they must compare CT images from different dates, perhaps in different disease stages. They must know how much a patient's bronchi are dilated, in which bronchus, or in which part of the lungs. Furthermore, they must compare other geometrical characteristics among different stages. A conventional method is to compare two CT datasets visually in side-by-side manner. However, workload for this procedure is extremely high. Moreover, the tree-structures from same patient in different disease stages are often not exactly same due to disease progression and other factors. Therefore, our objective is to construct a robust automatic mapping algorithm for the airway trees from a same patient in different disease stages. Then we assign geometrical information such as the cross-sectional area, curvature, and torsion to the respective edges, which can be easily used for assessment by physicians.
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Accelerated Molecular Design using Quantum Chemical Simulations and Deep Learning Models

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Key Words: *Molecular Design, Quantum Chemistry, Artificial Intelligence, Deep Learning, Surrogate Model*

Efficient methods for searching the chemical space of molecular compounds are needed to automate and accelerate the design of new functional molecules such as pharmaceuticals. Given the high cost in both resources and time for experimental efforts, computational approaches play a key role in guiding the selection of promising molecules for further investigation. Here, we construct a workflow to accelerate design by combining approximate quantum chemical methods [i.e., density-functional tight-binding (DFTB)], a graph convolutional neural network (GCNN) surrogate model for chemical property prediction, and a masked language model (MLM) for molecule generation. Property data from the DFTB calculations are used to train the surrogate model; the surrogate model is used to score candidates generated by the MLM. The surrogate reduces computation time by orders of magnitude compared to the DFTB calculations, enabling an increased search of chemical space. Furthermore, the MLM generates a diverse set of chemical modifications based on pre-training from a large compound library. We utilize the workflow to search for near-infrared photoactive molecules by minimizing the predicted HOMO-LUMO gap as the target property. Our results show that the workflow can generate optimized molecules outside of the original training set, which suggests that iterations of the workflow could be useful for searching vast chemical spaces in a wide range of design problems.

Bayesian Model Selection of Partial Differential Equations for Pattern Formation

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Key Words: *Pattern Formation, Partial Differential Equations, Bayesian Inference, Model Selection*

Partial differential equations (PDE) have been widely used to reproduce patterns in nature. To understand the mechanism of pattern formation, nonlinear PDEs have been employed for fluid convection[2], microphase separation of block copolymers[3], and crystals[4]. These PDEs may also be applied to pattern formation in biological systems[5]. Although a number of PDE models have been proposed, they rely on pre-request knowledge of physical laws and symmetries, and it requires significant efforts to develop a model reproducing the desired pattern. The challenge is quantitative and interpretable modelling of a complex phenomenon, which demands both developing a model and parameter estimation. The identification of a model equation is a recent key topic of machine learning and data science. Several methods have been proposed to derive PDEs from time-series data[6]. In this study, we propose the method to select a PDE model and its parameters to reproduce a given snapshot of a pattern, and from that, to get a physical insight of the target pattern[1]. We apply our method to nontrivial patterns, such as dodecagonal quasi-crystal, double gyroid, and Frank-Kasper structure, and we could successfully reproduce these patterns from the estimated PDE models.

We consider a pattern that is expressed by the scalar density field. We explorer a model to reproduce a target pattern at the steady state of an unknown model described by nonlinear PDEs. We consider a family of the models based on a phase-field crystal (PFC) model in which each model has different length scales. For a given target pattern, we estimate the appropriate number of length scales by estimating the best model, and also estimate the parameters in the model. The estimation is performed by the Bayesian model selection in which we compute the posterior distribution of parameters and marginal likelihood using the replica-exchange Monte Carlo (REMC) sampling. Our method is based on statistical inference, and therefore, it works for a noisy target and a target without ground truth.

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Bump Attractors and Waves in Networks of Integrate-and-Fire Neurons

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Key Words: Coherent Structures, Mathematical Neuroscience, Turbulence, Dynamical Systems.

Bump attractors are localised patterns observed in in vivo experiments of neurobiological networks. They are important for the brain's navigational system and specific memory tasks [1, 2]. A bump attractor is characterised by a core in which neurons fire frequently, while those away from the core do not fire. We uncover a relationship between bump attractors and travelling waves in a classical network of excitable, leaky integrate-and-fire neurons [3]. This relationship bears strong similarities to the one between complex spatiotemporal patterns and waves at the onset of pipe turbulence [4, 5]. We define and study analytical properties of the voltage mapping, an operator transforming a solution's firing set into its spatiotemporal profile. This operator allows us to construct localised travelling waves with an arbitrary number of spikes at the core, and to study their linear stability. A homogeneous "laminar" state exists in the network, and it is linearly stable for all values of the principal control parameter. We show that one can construct waves with a seemingly arbitrary number of spikes at the core; the higher the number of spikes, the slower the wave, and the more its profile resembles a stationary bump. As in the fluid-dynamical analogy, such waves coexist with the homogeneous state, are unstable, and the solution branches to which they belong are disconnected from the laminar state. We provide evidence that the dynamics of the bump attractor displays echoes of the unstable waves

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Computational Blood Flow Analysis of Arteriovenous Fistulas for Hemodialysis Patients

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Key Words: Arteriovenous Fistula, Hemodialysis, Disturbed flow, Regurgitation, Wall shear stress

Patient-specific computations are emerging extensively to assist hemodialysis patients in better assessing and planning surgical anastomosis. Over the last decades, end-stage renal disease (ESRD) has emerged as a severe clinical problem, leading to high morbidity rates. ESRD conditions are associated with impaired kidney function, for which hemodialysis procedures are strongly advised [1]. Such procedures require a well-functioning vascular access between the artery and the vein, known as an arteriovenous fistula (AVF). The hemodynamics characteristics within the AVFs depend greatly on patient-specific morphologies and flow conditions, which vary significantly between individuals.

This presentation analyzes blood flow dynamics for various three-dimensional AVFs for hemodialysis patients using CT scanning and phase-contrast MRI medical imaging data. Blood is modeled as a Newtonian fluid governed by unsteady, incompressible Navier–Stokes equations for computation. These governing equations have been solved numerically using stabilized finite element method [2], and details of the computational methods are described in [3]. In this study, we classified the considered AVFs as: *Splitting*, *Merging*, and *Almost one-way* cases, based on the regurgitation flow from the distal artery. We have computed several complex flow dynamics, pressure drops, and wall shear stresses. We have observed that the maximum inflows are confined to the distal vein near the anastomotic sites, for cases with regurgitation flow. In these cases, the pressure drop associated with disturbances in the main flow of the distal vein is also high. This regurgitation flow appears to be strongly associated with significant energy loss.

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Finite element analysis for a generalized Robin boundary value problem in a smooth domain

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Key Words: Generalized Robin Boundary Condition, Finite Element Method, Domain Perturbation

A generalized Robin boundary condition (GRBC) is one of the models appearing in coupled bulk-surface PDEs [2]. For example, [1] derived a reduced-order model for the fluid-structure interaction problem for blood flow in an arterial vessel by reducing the PDE describing the motion of a thin solid region—thus 3D—to the one defined on a fluid-solid interface which is 2D. The resulting equations, in a mathematically simplified form, have a feature represented by the GRBC.

In our previous work [3] we derived a weak formulation for the GRBC problem and established well-posedness as well as regularity properties on the level of PDE, assuming that the domain is smooth enough. We also provided some finite element analysis; however there we assumed that the domain is polygonal so that it can admit triangular meshes fitting its boundary exactly.

In the present study we treat a standard piecewise linear finite element method applied to the GRBC problem in a general domain with a curved boundary. Since a smooth domain is approximated by polygonal ones, we need to evaluate domain perturbation errors. We show that optimal error estimates are still available in this situation, which is the main result.

The novelty of this result is that the errors are evaluated in approximate domains in a more direct manner—thus may be useful for a practical purpose—than the ones used in [2, 4] where they compared approximate solutions with an exact one in the original smooth domain by introducing an abstract transformation which is not easy to compute in general.

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Hierarchical model reduction: a POD-based strategy to manage geometric bifurcations

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Key Words: Hierarchical model reduction, Proper orthogonal decomposition, Domain Decomposition

Hierarchical Model (HiMod) reduction proved to be an efficient and reliable tool to deal with directional phenomena [2, 1]. So far, the main field of application for such a model reduction procedure has been the modeling of the blood flow in arteries. The theoretical formalization of HiMod reduction in [3] inherently excludes geometric settings characterized by branches, such as bifurcation regions in hemodynamics. This limit prompted us to propose a specific strategy to overcome such an issue. The idea we pursue is based on the splitting of the domain into subdomains, in order to isolate the bifurcation from the rest. Then, to contain the whole computational cost, we solve the reference problem in the bifurcation by combining finite elements with a standard Proper Orthogonal Decomposition (POD), while resorting to a HiMod approximation along the branches. Finally, the different approximations are linked together through a domain decomposition procedure.

In this presentation, we adopt a standard scalar advection-diffusion-reaction model as reference problem to track the transport of a substance of interest in the blood (for instance, the contrast medium in a CT angiography). After detailing the proposed procedure, we will focus on the numerical assessment in order to highlight the efficiency and the accuracy of the methodology.

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Homological Features of Volumetric Images

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Key Words: *Imaging, Radiology, Homology, Lung CT*

Modern medical imaging techniques have enabled access to the interior of the human body in the form of not only 2D images but also 3D volumes. It is, however, not easy to utilise the 3D information, and analysis is often limited to a slice-by-slice investigation. We need a set of features for volumetric data to take full advantage of the 3D measurements.
On the one hand, radiomic features have been proposed to capture textural characteristics of a volume. They are computed from small patches of a volume and encode only local properties.
On the other hand, persistent homology provides computational machinery to extract the global structure of a volume. Although persistent homology is a promising tool that would complement the conventional radiomics, it is not yet widely used in medical image analysis, partly due to the lack of convenient software and the unusual form of its output as a multiset in the plane.
In this talk, we present our software, Cubical Ripser [1,2], for efficiently computing persistent homology of volumetric data.
We demonstrate its clinical relevance on abnormality quantification and detection in lung CT [3].

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Implementation of a Multi-Scale Model for Simulating Blood Flows in Circulatory Network

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Key Words: multi-scale model, one-dimensional arterial network, lumped-parameter models

Cardiovascular blood circulatory system serves as an important role in maintaining the normal operation of human life. Therefore, the pathological study and treatment of cardiovascular diseases attract researchers' interests. Mathematical models of the circulatory system which describe hemodynamic and vascular abnormalities have been recognized to be of great significance for this study and treatment.

In this work, blood circulation is numerically simulated by a multi-scale model which is constructed by coupling one-dimensional (1D) arterial network with lumped-parameter (0D) models[2]. 1D model, based on partial differential equations, aims to describe the detailed evolution of the cross-sectional area (A) and blood flow (Q) for each interested arterial segment, and that of mean pressure P consequently. 0D model, based on ordinary differential equations, describes the vascular subsystem corresponding to each peripheral artery. The combined 1D-0D multi-scale model can simulate hemodynamic and wave propagation characteristics of vascular system simultaneously in the time- and spatial-field. It is further assumed that the arterial tree is characterized by multi-branched arteries. At the bifurcations, flow conditions would be suitably matched with the conservation of mass flux and continuity of total pressure[1].

In computation, the boundary condition at the entrance of the arterial tree follows the action of heart. 1D and 0D models are solved by the two-step Lax-Wdndroff scheme and fourth-order Runge-Kutta method, respectively. The coupling of two models is numerically implemented at the spatial interfaces of two systems in a time-matching manner, and the derived equations are solved by using a Newton-Raphson method. Simulations of blood vessels with boundary conditions, and arterial networks with various bifurcations are presented in this study. It is shown how blood flows in the human arterial system including the circle of Willis. Furthermore, it has the potential to distinguish or predict the cerebrovascular states, such as occluded vessels, by investigating the effects of the blood flow patterns on cerebral outflows of time-dependent changes.

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Multiscale design and topology optimization of architected implants for bone replacement

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Key Words: *Topology optimization, Mechanical biocompatibility, Bone replacement implants, 3D printing,*

Architected materials can be designed to bring about clinical advantages over existing materials currently used in orthopaedics. In this talk, I will present a platform technology to develop 3D printed bone replacement implants with tailored lattice architecture of superior biomechanical performance. I will focus on key aspects pertaining to the multiscale modelling of manufacturing induced defects and topology optimization of representative implants, such as knee and cervical fusion cage. Emphasis will be placed on how to boost their mechanical biocompatibility to reduce bone resorption and achieve long-term functional performance.

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Sensitivity analysis of a partial hepatectomy hemodynamics model

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Key Words: computational hemodynamics, sensitivity analysis, partial hepatectomy, polynomial chaos expansion

Partial hepatectomy is the partial removal of the liver that is usually executed as a treatment option in liver cancer or for living donor transplantation. Exploiting the electric analogy to fluid flow, our team has developed a lumped parameter model to study the effect of partial hepatectomy on hemodynamics changes in the liver and the entire circulation [1]. This hemodynamics model evaluates - in a non-invasive way - the risk of postoperative portal hypertension, which may lead to post-hepatectomy liver failure, the leading cause of postoperative death.
This work studies *(i)* a propagation of variabilities from model input to output to investigate the main statistical moments of the outputs and the model reliability, and *(ii)* a sensitivity analysis (SA) study to identify the most significant parameters with respect to the main clinical output of interest. From a modeling viewpoint, these results allowed us to simplify the model by fixing model inputs that have negligible effect on the selected output. From a clinical viewpoint, this analysis provides a first step towards a better understanding of which patient-specific measurements are pivotal in the clinical routine to improve the quality of the numerical predictions. From a numerical viewpoint, we combined a selection algorithm due to physiological constraints with the polynomial chaos expansion (PCE) method [3]. In order to obtain only physiological outcomes we considered valid only the outcomes that comply with clinical indications. This selection induced some difficulties in the SA, due to the fact that the selected sample space was no more respecting the required hypothesis to apply the classic Saltelli algorithm [2]. To overcome this issue and to avoid a full MonteCarlo study, which would explode the number of simulations needed, we employ the PCE method on the physiological subspace, thus obtaining at a controlled computational cost the sensitivity indices. Finally, we completed a convergence study of this new SA exploratory method to verify the accuracy of such technique in the context of a partial hepatectomy hemodynamics model.

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Synthetic Q-Space Learning for Diffusion MRI Parameter Inference

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Key Words: *Diffusion MRI, Parametric Signal Models, Synthetic Q-Space learning*

Diffusion MRI (dMRI) can characterize and quantify the local properties of microstructures of the living organism such as the brain white matter [1]. The analysis is based on the parameters of various signal models of dMRI, such as diffusion tensor imaging (DTI), diffusion kurtosis imaging (DKI), neurite orientation dispersion diffusion imaging (NODDI), free-water imaging (FWI) and so on. One of the important features in those models is that anatomical structures are considered in the model. For example, parameters such as axon diameter and neurite orientation dispersion are included in the signal models. Consequently, the models become more complex and need more computational costs in parameter inference by conventional fitting methods.

Recent reports showed that machine learning approaches [2] are promising for inferring the parameters instead of fitting. Especially, training with synthetic data based on signal model equation and noise simulation, named synthetic Q-space learning (synQSL), showed great advantages and interesting characteristics [3]. In the synQSL scheme, the model parameters are randomly generated as gold standard in the practical range of the parameters first. Then, dMRI signal values are simulated by using signal model equation, and are contaminated by noise. A large quantity of pairs of gold standard parameters and simulated dMRI signals are prepared for training of a regressor used for parameter inference. The regressors can be chosen from the family of machine learning-based regressors, such as multi-layer perceptron (MLP), random forest and so on. The major advantages of synQSL are robustness and fast computation. It is known that the robustness depends on the training noise level, and noise level match between training data and test data yields optimal robustness.

In this talk, the basics of dMRI parameter inference by using synQSL are introduced with examples of parameter inference in models of DTI, DKI, NODDI and FWI. Also, the characteristics and current issues of the approach are discussed.

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Uncertainty Related to the Use of Doppler Flow Waveforms as Inflow Boundary Conditions in Coronary Arteries Blood Flow Simulations

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Key Words: *computational hemodynamics, uncertainties, coronary arteries, wall shear stress*

Introduction: coronary arteries, supplying blood to myocardium are among the most clinically relevant arteries and the role that local hemodynamics play in atherosclerosis initiation and progression is well established [1]. In recent years the combination of computational fluid dynamics (CFD) and medical imaging has allowed to precisely profile wall shear stress (WSS) features in realistic coronary artery models with spatial and temporal accuracy that cannot be obtained with standard clinical measurement [2]. However, the clinical use of CFD simulations is still hampered by those assumptions/idealizations which each model-based strategy necessarily introduces, and which represent a source of uncertainty. One main source of uncertainty in modelling coronary hemodynamics is represented by the inflow boundary conditions (BCs), because of the paucity of information available. In this context the aim of this study was to investigate the budget of uncertainty on WSS profiles associated with blood velocity waveforms in coronary arteries as given by intravascular Doppler flow measurements when the latter are used as inflow BCs.

Methods: the geometry of 7 left anterior descending (LAD) and 7 right coronary arteries (RCA) were reconstructed from angiographic projections using a commercial software (QAngio XA bifurcation, Medis Medical imaging). Then geometries were discretized, and the governing equations of unsteady-state fluid motion were numerically solved by means of the finite volume-based commercial code Fluent (Ansys Inc.) by imposing two different inflow BCs: (1) patient-specific velocity waveforms from intravascular Doppler flow measurements and (2) generalized velocity waveforms obtained averaging patient-specific Doppler flow waveforms, scaled to the same cycle-average flow rate obtained from the patient-specific Doppler flow waveforms. The impact of inflow BC strategy was evaluated in terms of WSS profile accounting for WSS magnitude (time averaged WSS, TAWSS), pulsatility (oscillatory shear index, OSI), and topological features (topological shear variation index, TSVI) [3]. The impact on WSS-based descriptors was evaluated in terms of surface averaged values, percentage of surface area exposed to low TAWSS and high OSI and TSVI, and colocalization of surface area by means of similarity index (SI).

Results and conclusions: the main differences emerged between WSS obtained adopting the two different inflow BC strategies can be summarized as follows: (1) significant differences were observed in terms of surface averaged values for TAWSS ($p=0.002$), OSI ($p<0.001$), and TSVI ($p<0.001$); (2) a strong, significant linear correlation was observed for TAWSS ($r=0.98$, $p<0.001$), OSI ($r=0.94$, $p<0.001$), and TSVI ($r=0.80$, $p<0.001$); (3) no significant differences emerged on percentage surface area exposed to low TAWSS, and high OSI and TSVI; (4) colocalization was very high for TAWSS (SI=0.98[0.97-0.99]), and moderate for OSI (SI=0.66[0.50-0.81]) and TSVI (SI=0.60[0.48-0.71]). The findings of this study suggest that adopting patient-specific rather than generalized Doppler flow data as inflow BC in coronary hemodynamics simulations might influence more WSS directionality and topological features than WSS magnitude.

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Well-posedness of One-dimensional Models of Blood Flow in Arteries

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Key Words: One-dimensional model, Reduced model, Well-posedness

One-dimensional (1D) models of blood flow are useful reduced models of the cardiovascular system and they are frequently applied in numerical simulations of blood flow in arteries. See [2] for example. Though models are highly simplified with respect to the local dynamics, they bring us reliable results at a low computational cost. To perform numerical simulation, it is required to derive the well-posed formulations with appropriate boundary and compatibility conditions. The aim of this study is to provide a mathematical study for the 1D model that will give an essential contribution to numerical simulations.

We consider the Navier–Stokes equations for an incompressible fluid flow in a simple compliant tube that is a model of the artery. An asymptotic analysis gives a nonlinear nonsymmetric hyperbolic system of partial differential equations, which we call the 1D system, for the area of a cross-section A and the mass flux Q across the section. We pose a constructive assumption on the pressure. That is, the pressure is assumed to be represented in terms of A. The 1D system contains a momentum-flux correction coefficient $\alpha \geq 1$. The case $\alpha > 1$ is physiologically interestsing, but mathematical study are often resctricted to the case $\alpha = 1$.

For the mathematical well-posedness of the 1D system, we usually refer to [1], where the unique existence of a time-global smooth solution is proved. However, the work [1] studied only the case $\alpha = 1$. The purpose of the present paper is to establish the well-posedness of the 1D system. In particular, we prove that under some suitable compatibility conditions there exists a $T > 0$ and a unique solution $(A,Q) \in C^0([0,T];H^2(\mathbb{R},\mathbb{R}^2)) \cap C^1([0,T];H^1(\mathbb{R},\mathbb{R}^2))$ of the 1D system with any $\alpha \geq 1$. Therein, $H^s(\mathbb{R},\mathbb{R}^2)$ stands for the Sobolev space in the L^2 sense. To accomplish the purpose, we apply an abstract theory of Kato [3].

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A Further Extended Range of Stable Flux Reconstruction Schemes in One Dimension, Triangles, and Polygons

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Key Words: High-order, flux reconstruction, summation-by-parts

We present new approaches for developing stable flux reconstruction (FR) [2] schemes in multiple dimensions, building on the previous work of Vincent et al. [4]. Starting in one-dimension, we explore the use of summation-by-parts (SBP) techniques [3], formulating methods to identify new multi-parameter correction functions. We then extend the approach to higher dimensions and tackle the more complex task of applying symmetry constraints for these elements. A new range of stable schemes will be presented for triangles, a subset of which are those of Castonguay et al. [1]. Finally, we will go on to present the new class of methods for both quadrilateral, and, for the first time, hexagonal elements.

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Application of *A Posteriori* Slope Limiter to Ideal Magnetohydrodynamics Simulation

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Key Words: *Slope Limiter, Magnetohydrodynamics, MUSCL, Finite Volume Method*

Introduction: Magnetohydrodynamics (MHD), which takes into account the interaction between magnetic fields and plasmas, is used in a wide range of research fields such as astrophysics, space engineering, and nuclear fusion. In MHD simulations using the finite volume method, the monotonic upstream-centered scheme for conservation laws (MUSCL) is a very popular method for higher-order accuracy. In the conventional MUSCL, stable computation is achieved by adding a slope limiter to the region where overshoot/undershoot is likely to occur. However, this procedure may result in limiting the slopes more than necessary. To address this problem, we proposed "*a posteriori* limiter" (hereafter referred to as "Post Limiter") in gas dynamics simulations [1], which was a modification of the conventional MUSCL calculation procedure: By accepting slight overshoot/undershoot near discontinuities, this method has been confirmed to be effective in improving both resolution and convergence, and suppressing undesired oscillations in smooth regions. In this study, we extend the Post Limiter to MHD simulations involving more types of discontinuities (e.g., rotational discontinuity, fast/slow shock wave) than gas dynamics, and show its performance by one- and two- dimensional MHD tests.
Proposed Method: The Post Limiter does not limit the slope for weak shocks (pre-shock Mach number less than 1.36), even if the un-limited values do not satisfy the discrete maximum principle (see Ref. [1] for details). In the original Post Limiter, the pressure ratio was used to evaluate the shock strength. In gas dynamics, this evaluation method is appropriate since the pressure ratio corresponds to the pre-shock Mach number. In MHD, however, there is no corresponding relation between the pressure ratio and the Mach number of the pre-shock. Thus, in this study, the evaluation method of the Post Limiter is modified to consider the tangential component of the magnetic field.
Numerical Results: In many smooth regions, the Post Limiter achieves higher resolution than conventional calculation procedures. Although overshoot/undershoot occurs near the discontinuities, no further adverse effects are observed. For some tests, we have confirmed that Post Limiter suppresses oscillations and is closer to the reference than the 5-order monotonicity preserving (MP5) scheme, an expensive higher-order scheme (MP5 requires about 1.95 times more computation time than the conventional MUSCL for one-dimensional tests).
Conclusion: Numerical tests have shown the performance of the Post Limiter in MHD simulations. The proposed method provides resolution improvement by accepting overshoot/undershoot, and in one-dimensional tests, the resolution is about four times higher than the conventional MUSCL in many regions. In addition, the Post Limiter can be implemented for conventional MUSCL with only a few modifications to the computational code. Therefore, considering a marginal increase in computation time (about 1.25 times for one-dimensional tests), the Post Limiter is more effective than the use of a finer computational mesh. In the final paper, we will discuss in more detail the conditions necessary to extend Post Limiter to MHD simulations.

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Extending High-Order Spectral Difference Method with Constrained Transport to Resistive Compressible Magnetohydrodynamic Simulations on Unstructured Grids

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Key Words: *Spectral Difference, High-Order, Computational Magnetohydrodynamics, Unstructured Grids*

High-Order Spectral Difference method with Constrained Transport (SDCT) is proposed in [1] to solve compressible magnetohydrodynamic (MHD) equations. This approach can maintain the divergence-free constraint to the accuracy of machine-precision error throughout the simulations. And the additional computational cost is less than 1/8 compared with that without constrained transport. However, it can only be applied to ideal MHD equations on structured rectangular meshes. In this paper, we extend the original SDCT method to resistive MHD equations by adding an artificial resistive term directly acting on the magnetic potential instead of the magnetic field. This approach does not affect the smoothness of the solution and provides enough dissipation to damp spurious discontinuity of the magnetic field. This resistive version of SDCT method can be then applied to simulations of magnetic reconnection, large-scale magneto-convection, etc. Moreover, the solution accuracy is tested when the computational grids are unstructured. It is found that the high-order accuracy is still preserved. Meanwhile, the divergence-free constraint is kept under some threshold and the divergence error does not accumulate with time integration. The divergence error is proved to decay exponentially with the reduction of the mesh size.

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High-Order Hybridizable Discontinuous Galerkin Methods for Computational Fluid Dynamics with Applications to Multiphysics Problems

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Key Words: Hybridizable discontinuous Galerkin, Compressible flows, Magnetohydrodynamics, Fluid-structure interaction, Finite element coupling

In this contribution, we present high-order hybridizable discontinuous Galerkin (HDG) formulations for computational fluid dynamics and recent applications to multiphysics problems. A novel weakly compressible fluid formulation [1], featuring the velocity and the pressure as primal variables, is first introduced. Its superior features with respect to density–momentum-based approaches [2] are highlighted on a simple example, especially regarding the good conditioning of the resulting linear system over a wide range of compressibility levels. Such flow solver is then combined with Maxwell's equations for the solution of magnetohydrodynamic problems [1]. The convergence properties of the resulting coupled multiphysics problem are demonstrated on several numerical examples on structured and unstructured meshes and at low and high Hartmann numbers.

A strategy to couple HDG and standard finite element discretizations is also presented [3]. Devising different spatial discretizations can be of particular interest in the context of multiphysics simulations, as well as for multimaterial problems in which different regions of the computational domain feature distinct physical properties. The proposed method exploits the definition of the numerical flux and the trace of the solution on the mesh skeleton to impose the coupling conditions solely in the global problem by means of Nitsche's method. The key advantage is the minimal intrusiveness in terms of computer implementation that makes it suitable to be integrated in existing finite elements libraries. This strategy is thus successfully applied for the solution fluid-structure interaction problems [2].

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High-Order Implicit Shock Tracking for Compressible Viscous Flows

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Key Words: Shock Fitting, Discontinuous Galerkin, PDE-Constrained Optimization

Reference link: https://www.wccm2022.org/submission.html

Shock tracking, as an alternative method to shock capturing, aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter-element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or extensive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features. In previous work [1, 2], we introduced the High-Order Implicit Shock Tracking (HOIST) method that recasts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conservation, stability, and high-order accuracy. By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh.

In this work, the HOIST method is further extended to simulate viscous flows. To accommodate for the viscous shocks (sharp gradients), a continuation strategy for viscosity is integrated into the SQP solver to promote mesh compression towards the sharp gradient. In contrast to the inviscid problems where shocks are represented by inter-element solution jumps, a layer of compressed elements provides sufficient resolution for the sharp solution gradient. The method is demonstrated on a series of increasingly complex viscous, compressible flows.

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On Numerical Instabilities of High-Order Shock-Capturing schemes for strong shocks

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Key Words: High-order Methods, Shock Capturing, Shock Instability, Hypersonic

The accurate and robust prediction of hypersonic heating is still challenging. One of the primary difficulties is robust capturing of strong shock waves in hypersonic flows[1, 2]. At present, shock-capturing schemes used in hypersonic flow simulations often encounter numerical shock instabilities, which greatly limits the accuracy and efficiency of hypersonic heating computations. For high-order shock-capturing schemes, the shock instability problem is even more difficult to deal with[3, 4]. In the current study, a matrix stability analysis method[5] is developed for high-order WENO schemes to quantitatively analyze the shock instability problem. The mechanism of hypersonic numerical shock instability for third-order, fifth-order and seven-order WENO schemes are presented. Results of numerical stability analysis show that the shock instability is not only closely related to the upstream Mach number, but also to the reconstruction stencil and the numerical dissipation of WENO schemes. The effect of the computational grids on shock wave stability is also presented. Such an analysis is useful for developing more robust and reliable high-order methods for hypersonic heating computations.

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The Importance of Temporal Adaptation in High-Order Unsteady Simulations

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Key Words: Unsteady adjoint, Output-based adaptation, Arbitrary Lagrangian Eulerian, Discontinuous Galerkin

The combination of high-order spatial schemes and output-based mesh adaptation has yielded a robust steady simulation approach that produces highly accurate output predictions even in the presence of singular solution features. Less effort has been devoted to unsteady problems, for which high-order spatial methods are paired with high-order temporal schemes. In the presence of non-smooth temporal solutions or output definitions, which are commonplace in practical engineering problems, high-order accuracy in time can be difficult to obtain. We present a study of the importance of output-based adaptation to address these difficulties. The demonstration suite consists of unsteady fluid dynamics simulations of the compressible Navier-Stokes equations on deforming domains [2], discretized with the discontinuous Galerkin method in space and high-order multi-stage methods in time, with motion that is reasonably smooth but not infinitely differentiable. Spatial and temporal output-based adaptation is performed using discrete-in-space and continuous-in-time adjoints [1]. On a benchmark problem suite [3], we show that proper isolation of temporal singularities is important for high-order accuracy, and that it is achievable within a space-time adaptive framework.

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A particle dynamics model for coarsening process of Cahn–Hilliard equation

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Key Words: model order reduction, Cahn–Hilliard equation, particle model, coarsening process

The Cahn–Hilliard equation [1] is a model equation to describe phase separation phenomena, which is notorious for its difficulty in obtaining stable numerical solutions. The phase separation phenomena consist of two processes: rapid separation process and slow coarsening process. We focus on the latter. There are several previous studies on reduction models for coarsening process. Argentina et al. [2] construct some mathematical representations to approximate solutions to Cahn–Hilliard equation and investigate coarsening process via the representations.

This work proposes a reduction model for Cahn–Hilliard equation's slow coarsening dynamics process. The model is to mimic the movement of multiple concentrated phases ("bubbles"). To design the model, we assume that a "force" governs the movement and that the force depends on the distance between bubbles. Via some preliminary numerical computations, we observed that these assumptions seem to be satisfied virtually for the movement of similar two bubbles in two-dimensional problems. Furthermore, we found that an inverse square law governs the movement. In addition, we also assume that the "work," which is the application of force along with a displacement, equals the variation of total energy. In the presentation, we will discuss the validity of the proposed model through some numerical computations.

We note that the numerical computation has been conducted for only two-dimensional problems. We have to investigate if the proposed model is valid for one- or three-dimensional problems. Of course, we also plan to design some reduction models for the rapid separation process.

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Enforcing physical structure in Bayesian learning of dynamical systems: stability and energy conservation

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Key Words: Bayesian Inference, Data-driven modeling, Structure-preserving learning

We describe a Bayesian probabilistic formulation for system identification of dynamical systems. The approach uses an approximate marginal Markov Chain Monte Carlo algorithm to directly discover a system from data. Here, we demonstrate that the posterior distribution simultaneously accounts for unknown parameters, model form uncertainty, and measurement noise. As a result of this feature, we show that our approach becomes more robust than current state-of-the-art methods that rely on heuristic least-squares optimization objectives. Our approach is also approximation-format agnostic and works with both linear and nonlinear dynamical system parameterizations. We show numerous examples demonstrating that we outperform more standard operator inference and vector-field inference approaches when data becomes noisy.

Next we extend our approach to direct identification of system Hamiltonians. Here, our approach improves upon existing approaches by encoding the fact that the data generating process is symplectic directly into our learning objective. This objective is the log marginal posterior of a probabilistic model that embeds a symplectic and reversible integrator within an uncertain dynamical system. We demonstrate that the resulting learning problem yields dynamical systems that have improved accuracy and reduced predictive uncertainty compared to existing state-of-the-art approaches. Simulation results are shown on several Hamiltonian benchmarking systems.

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Hamiltonian Operator Inference: Physics-preserving Learning of Reduced-order Models for Hamiltonian Systems

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Key Words: Structure-preserving model reduction; Hamiltonian systems; Physics-informed machine learning; Data-driven modeling; Operator inference

This work presents a nonintrusive physics-preserving method to learn reduced-order models (ROMs) of Hamiltonian systems. Traditional intrusive projection-based model reduction approaches utilize symplectic Galerkin projection to construct Hamiltonian reduced models by projecting Hamilton's equations of the full model onto a symplectic subspace. This symplectic projection requires complete knowledge about the full model operators and full access to manipulate the computer code. In contrast, the proposed Hamiltonian operator inference approach embeds the physics into the operator inference framework to develop a data-driven model reduction method that preserves the underlying symplectic structure. Our method exploits knowledge of the Hamiltonian functional to define and parametrize a Hamiltonian ROM form which can then be learned from data projected via symplectic projectors. The proposed method is 'gray-box' in that it utilizes knowledge of the Hamiltonian structure at the partial differential equation level, as well as knowledge of spatially local components in the system. However, it does not require access to computer code, only data to learn the models. Our numerical results demonstrate Hamiltonian operator inference on a linear wave equation, the cubic nonlinear Schroedinger equation, and a nonpolynomial sine-Gordon equation. Accurate long-time predictions far outside the training time interval for nonlinear examples illustrate the generalizability of our learned models.

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Learning Low-dimensional Quadratic Embeddings of High-fidelity Nonlinear Dynamics using Convolutional Autoencoders

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Key Words: Model Order Reduction, Scientific Machine Learning, Quadratic Embedding, Autoencoder

Learning dynamical models from data plays a vital role in engineering design, optimization, and predictions. Building models describing dynamics of complex processes (e.g., weather dynamics, reactive flows, brain/neural activity, ...) using empirical knowledge or first principles is frequently onerous or infeasible. Moreover, these models are high-dimensional but spatially correlated. It can, however, be often observed that the dynamics of high-fidelity models evolve in low-dimensional manifolds. Furthermore, it is also known that for sufficiently smooth vector fields defining the nonlinear dynamics, a quadratic model may be able to describe the dynamics of the model accurately in an appropriate coordinate system, conferring to the McCormick relaxation idea in nonconvex optimization. Here, we aim at finding a low-dimensional embedding of high-fidelity dynamical data, similar to [2], ensuring a simple quadratic model to explain its dynamics. To that aim, this work leverages deep learning to identify low-dimensional quadratic embeddings for high-fidelity dynamical systems. Precisely, we identify the embedding of data using an autoencoder [3] to have the desired property of the embedding. We also embed a Runge-Kutta method as in [1] to avoid the often challenging time-derivative computations. We illustrate the ability of the approach by a couple of examples, arising in describing flow dynamics and the oscillatory tubular reactor model.

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Probabilistic Superiority of Stochastic Symplectic Methods via Large Deviations Principle

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Key Words: *Stochastic Symplectic Methods, Superiority, Large Deviations Principle, Rate Function, Asymptotical Preservation*

Plenty of numerical experiments show that stochastic symplectic methods are superior to non-symplectic ones especially in long-time computation, when applied to stochastic Hamiltonian systems. In this talk, we attempt to give an explanation on the superiority of stochastic symplectic methods by means of large deviations principle. We prove that stochastic symplectic methods are able to asymptotically preserve the large deviations principles for some observables of the exact solution, while non-symplectic ones do not. This indicates that stochastic symplectic methods are able to preserve the asymptotic results on rare event probabilities of the original system, and may provide an effective approach to approximating rate functions of large deviations principles.

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Quantifying the error in the numerical integration of ODEs based on isotonic regression

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Key Words: Model reduction, uncertainty quantification, structure-preservation

A system of ordinary differential equations (ODEs) is a fundamental tool for modelling a dynamical system. ODE models often include unknown system parameters or unknown initial states, and thus, estimating them is a fundamental task in, for example, data assimilation. The task usually requires solving ODEs numerically, and thus, unless the numerical computation is sufficiently accurate, the estimation is biased due to the error in numerical integration. Recent studies suggest that quantifying the forward uncertainty, i.e. the error in numerical integration, would be beneficial in this context [1]. Most of them assume a statistical model for the error, but it is usually quite large because the size is proportional to the system dimension times the number of time points, such as the number of observations or time steps of numerical integration. Therefore, it is essential to reduce the size of the statistical model while preserving the structure of the error behaviour. This talk presents an approach for this kind of model reduction. The key idea is to use generalised versions of isotonic regression, and the cost for the forward uncertainty quantification based on our approach is negligible compared to the single numerical integration of ODEs.

This talk is based on our recent papers [2, 3].

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Structure preserving semibalanced truncation of port-Hamiltonian systems

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Key Words: Structure preserving model reduction, balanced truncation, nonlinear systems, port Hamiltonian systems

Many physical systems can be represented as port-Hamiltonian systems (PHSs) [1], and various control methods utilizing the PH structure have been developed. Nowadays, models of physical systems can easily be high dimensional, e.g., large scale circuits, discretized PDE models, such as from flexible beams, etc. To simplify analysis or control of such systems by obtaining the benefit from the structure of a PHS, it is natural to develop a model reduction method preserving the PH structure. However, the traditional nonlinear balanced truncation method proposed by [2] does not preserve the PH structure. In this talk, we establish a balancing procedure for PHSs based on the controllability function and the internal energy given by the Hamiltonian, i.e., a combination of balancing and modal analysis. That is, for standard balancing [2], the controllability and observability Gramians are used, whereas in modal analysis the eigen modes of the system related to the internal energy are considered [3]. To the best of our knowledge, this has not been done elsewhere. When using such procedure for truncation, the port Hamiltonian structure is preserved naturally, whereas this is not the case in any other balancing procedure.

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Structure-Preserving Model Order Reduction on Manifolds

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Key Words: Model Order Reduction, Structure-Preserving, Differential Geometry

Model Order Reduction (MOR) with non-linear approximants has been introduced in various contexts, e.g. [1, 2, 3]. Following the terminology in [2], we call this approach MOR on Manifolds whereas MOR with linear approximants is referred to as classical MOR. The motivation of MOR on Manifolds is to apply MOR to systems that cannot be sufficiently reduced with classical MOR due to slowly decaying Kolmogorov n-widths, e.g. for linear advection [4]. To our best knowledge, none of the previous work has introduced this formulation in terms of a differential geometric framework. In this talk, we fill this gap and present the theory of MOR on Manifolds from the viewpoint of basic differential geometry. This contribution firstly connects two fields in mathematics, MOR and differential geometry. Moreover it provides a unified framework how to extend existing techniques for structure-preserving classical MOR to MOR on Manifolds for Lagrangian systems, Hamiltonian systems and other structures. The newly introduced connection gives rise to innovative ideas how to extend the training of the non-linear approximants, e.g. by including tangent information in the training process. We investigate such techniques in a numerical experiment for the one-dimensional Burger's equation.

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Structure-Preserving Model Reduction for Dissipative Differential Equations

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Key Words: Differential Equations, Structure-Preserving Numerical Methods, Model Reduction

In this talk, we consider numerical computation of dissipative gradient systems, such as Hamiltonian systems with friction, and systems that arise as discretizations of certain dissipative partial differential equations (such as the diffusion equation, or the Cahn–Hilliard equation for phase separation problems.) Such systems are often equipped with some energy functional that decays with time, which is important in that it controls asymptotic behavior of solutions.

The energy decay property could be preserved by "structure-preserving numerical methods." Their use is often preferred for better qualitative behaviors of the solutions and the stability of the numerical computations themselves. Structure-preserving methods are, however, in many cases fully-implicit, and prohibitive as is for large systems. It encourages us to introduce some model reduction techniques (for example, the proper orthogonal decomposition [1]), but it in turn generally destroys the important mathematical structure (the gradient structure, in the present case), which makes the overall strategy very problematic.

In this talk, we show a new structure-preserving model reduction technique for dissipative gradient systems, which successfully reduces the size of the system without destroying the gradient structure and the negative semi-definiteness of the preceding matrix. The technique is partially inspired by an existing technique for Hamiltonian systems (without friction) [2], but provides more general guiding principle for structure-preservation. With some numerical examples we illustrate that in fact such a structure-preserving model reduction provides us efficient, stable numerical computations.

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Structured Interpolatory Model Reduction of Nonlinear Dynamical Systems

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Key Words: Interpolation, Bilinear Systems, Quadratic Systems, Projection, Structured Interpolation

Interpolatory methods are one of the most widely used techniques for model reduction of large-scale dynamical systems [1]. In the case of linear dynamical systems, transfer function of the resulting reduced model interpolates that of the full (original) model at selected points in the complex plane. In many applications, the original system has a physical structure that needs to be retained in the reduced model so that the reduced model is physically meaningful. These structures range from the classical mass-spring-damper formulations to internal delays and more. For linear dynamics, based on the concept of generalized coprime factorization [2], structure-preserving interpolation has been extended to a wide class of structures so that the reduced model not only provides interpolation but also retains the underlying physical structure. In [3], these ideas has been recently extended bilinear dynamical systems, a special class of nonlinear dynamical systems.

In this talk, we will focus on quadratic-bilinear dynamical systems, a prominent class of nonlinear dynamical systems arising a wide range of applications. We will develop the concept of structured generalized transfer functions for quadratic systems and derive the necessary subspace conditions on the model reduction bases so that the reduced quadratic-bilinear system has the same physical structure/meaning as the original one and satisfies a variety of interpolation conditions on the leading subsystem transfer functions. We will illustrate the the underlying theory on various structured nonlinear models.

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Symplectic Model Reduction of Hamiltonian Systems on Nonlinear Manifolds

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Key Words: Model reduction on manifolds, Hamiltonian systems, convolutional autoencoders.

Traditional model reduction techniques project the governing equations onto linear subspaces of the high-dimensional state-space. This works well if the underlying problem admits fast decaying Kolmogorov-n-widths. However, for problems with slowly decaying Kolmogorov-n-widths such as certain transport-dominated problems [1], classical linear-subspace reduced order models (ROMs) of low dimension might yield inaccurate results. Thus, the reduced space needs to be extended to more general nonlinear manifolds. Moreover, as we are dealing with Hamiltonian systems, it is crucial that the underlying symplectic structure is preserved in the reduced model, see [2, 3].
To the best of our knowledge, existing literatures addresses either model reduction on manifolds or symplectic model reduction for Hamiltonian systems, but not their combination. In this talk, we bridge the two aforementioned approaches by providing a novel projection technique called *symplectic manifold Galerkin*, which projects the Hamiltonian system onto a symplectic nonlinear manifold such that the reduced model is again a Hamiltonian system. We derive analytical results such as stability, energy-preservation and a rigorous a-posteriori error bound. In addition, we propose a computationally practical approach to obtain a symplectic reduced manifold. To this end, we construct a weak symplectic convolutional autoencoder. We provide numerical results for a linear wave equation for which a slow decay of the Kolmogorov-n-width can be observed, see e.g. [4, 5].

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A Decoupled, Linear, And Unconditionally Energy Stable Finite Element Method For A Two-Phase Ferrohydrodynamics Model

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Key Words: *Ferrohydrodynamcis; Two-phase; Phase-field; Unconditional energy stability, Magnetic field.*

Abstract: In this talk, we present numerical approximations of a phase-field model for two-phase ferrofluids, which consists of the Navier-Stokes equations, the Cahn-Hilliard equation, the magnetostatic equations, as well as the magnetic field equation. By combining the projection method for the Navier-Stokes equations and some subtle implicit-explicit treatments for coupled nonlinear terms, we construct a decoupled, linear, fully discrete finite element scheme to solve the highly nonlinear and coupled multi-physics system efficiently. The scheme is provably unconditionally energy stable and leads to a series of decoupled linear equations to solve at each time step. Through numerous numerical examples in simulating benchmark problems such as the Rosensweig instability and droplet deformation, we demonstrate the stability and accuracy of the numerical scheme.

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A Discontinuous-Galerkin-in-Time Framework for Multirate Time Integration of Interface-Coupled Problems

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Key Words: multirate, multidomain, time stepping

A framework is presented to design multirate time stepping algorithms for two dissipative models with coupling across a physical interface. The coupling takes the form of boundary conditions imposed on the interface relating the solution variables for both models to each other. The multirate aspect arises when numerical time integration is performed with different time step sizes for the component models. We describe a unified approach to develop multirate algorithms for these problems. This effort is pursued though the use of discontinuous-Galerkin time stepping methods, acting as a general unified framework, with different time step sizes. The two models are coupled across user-defined intervals of time, called *coupling windows*, using polynomials that are continuous on the window. The coupling method is shown to reproduce the correct interfacial energy dissipation, discrete conservation of fluxes, and asymptotic accuracy. Also, the method could provide a limit for the total communication needed between components, independent of the number of time steps on a coupling window. In principle, methods of arbitrary order are possible. As a preliminary step, we focus on the presentation and analysis of monolithic methods for advection-diffusion models coupled via generalized Robin-type conditions. The monolithic methods could be computed using a Schur-complement approach. We also discuss some recent progress for partitioned algorithms and different types of coupling conditions.

A mathematically rigorous and physically consistent approach to the treatment of imperfect interfaces with nonlocal models

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Key Words: *Interface problems, imperfect interfaces, nonlocal models, nonlocal mechanics, asymptotic behavior of solutions.*

Nonlocal, integral models have become viable alternatives to partial differential equations (PDEs) when the effects of long-range interactions affect the global behavior of a system. As an example, in continuum mechanics, nonlocal equations accurately model multiscale effects and anomalous behavior such as discontinuities and singularities in the solution.
The presence of long-range interactions and the integral nature of nonlocal operators create several modeling and computational challenges that may hinder the usability of nonlocal equations. A major challenge is the treatment of interfaces; while in the classical setting an interface is a sharp entity separating two domains, in the nonlocal setting an interface is a thick layer between domains. This fact makes the treatment of interface conditions for the solution and its flux a nontrivial problem.
Building on previous efforts by the same authors focused on the treatment of "perfect interfaces" (for which the solution and the flux are continuous through the thick interface), we propose a novel approach for the treatment of "imperfect interfaces", i.e. interfaces that feature jumps in the solution and in the flux.
Our approach is mathematically rigorous, in the sense that the resulting interface problem is well-posed, and physically consistent. The latter statement, in the context of nonlocal models, implies that when the extent of the nonlocal interactions vanishes, the nonlocal interface problem and its solution converge to their classical counterparts, i.e. to the solution of the corresponding PDE.
The applicability of this method and our theoretical findings are illustrated via several one- and two-dimensional numerical tests.

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A nonlocal gradient for black-box optimization with its applications to data-driven discovery and design

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Key Words: Optimization, Inverse Problems, Model Discovery

The problem of minimizing multi-modal loss functions with a large number of local optima frequently arises in model calibration, architecture design and machine learning problems. Since the local gradient points to the direction of the steepest slope in an infinitesimal neighborhood, an optimizer guided by the local gradient is often trapped in a local minimum. To address this issue, we develop a novel nonlocal gradient to skip small local minima by capturing major structures of the loss's landscape in black-box optimization. The nonlocal gradient is defined by a directional Gaussian smoothing (DGS) approach. The key idea of DGS is to conducts 1D long-range exploration with a large smoothing radius along d orthogonal directions in $\mathbb{R}^d$, each of which defines a nonlocal directional derivative as a 1D integral. Such long-range exploration enables the nonlocal gradient to skip small local minima. The d directional derivatives are then assembled to form the nonlocal gradient. We use the Gauss-Hermite quadrature rule to approximate the d 1D integrals to obtain an accurate estimator. We demonstrate the superior performance of our method in several benchmark tests as well as data-driven discovery and design problems.

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Comparison of Methods for Coupling a Lagrangian Discrete Element Sea Ice Model to an Eulerian Ocean Model

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Key Words: Discrete element method, particle to grid coupling, sea ice, ocean

Coupled Earth system models require methods for accurate and conservative transfer of fields between submodels such as sea ice and ocean. Typically, sea ice and ocean submodels are solved with Eulerian PDE-based methods that are often discretized on the same underlying grid, which significantly simplifies data transfer between submodels. A new sea ice model, the Discrete Element Model for Sea Ice (DEMSI), is under development that relies on a Lagranigan particle-based discretization. DEMSI treats collections of ice floes as Lagrangian particles that interact through contact forces and their trajectories are determined by directly integrating the equations of motion. In contrast to standard Eulerian continuum models of the sea ice cover, this method enables the capture of the anisotropic sea ice deformation and fracture in response to ocean and atmospheric forcing. Integrating this type of Lagrangian model into a coupled Earth system model with a traditional Eulerian PDE-based ocean code requires new methods for accurate and conservative interpolation from discrete particles onto grids.

We will describe two approaches for coupling a discrete element sea ice model to an Eulerian ocean model discretized on a global Voronoi grid. In the first approach, we use a geometric interpolation method where intersections between Voronoi cells associated with Lagrangian sea ice particles and ocean grid cells are used to define interpolation weights between the particles and grid cells. A similar method has already been implemented within DEMSI for particle-to-particle remapping applications [1]. The second method utilizes a moving least squares approach implemented with the Compadre Toolkit [2]. A comparison of the accuracy and conservation properties of both methods will be presented.

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Design and evaluation of a waveform iteration–based approach for coupling heterogeneous time stepping methods via preCICE

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Key Words: Coupled problems, High-order time stepping, Multi-rate time stepping, Black-box coupling

For multiphysics simulations the robust and accurate coupling of different simulation codes is often required. Code coupling libraries, such as preCICE [1], allow the user to easily couple codes following a data-driven black-box approach, which ensures high flexibility and ease-of-use. However, the coupling of simulation codes that are working on different time-scales or using different time stepping schemes remains a big challenge [2].

To be able to combine the black-box coupling of preCICE with heterogeneous time stepping methods we designed a waveform iteration-based coupling scheme [3]. Additionally, we developed a software to facilitate the coupling of the off-the-shelf finite element solver FEniCS with preCICE – a so-called adapter [4].

In this talk, we present how these two components – the waveform iteration-based coupling scheme and the FEniCS-adapter – are combined to be used in a simulation setup that is close to a real application. This allows us to solve coupled problems with heterogeneous time stepping methods or time-scales in FEniCS. We introduce a test case to assess the accuracy of the whole software stack. With the overall architecture and a scheme for thorough evaluation in place, this marks a starting point for applying the proposed methodology to more complex problems.

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Fourth-Order Accurate Partitioned Schemes for Conjugate Heat Transfer and Advection

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Key Words: Partitioned Solvers, Conjugate Heat Transfer, Incompressible Flow

Here we discuss the development and analysis of fourth-order accurate partitioned solvers for conjugate heat transfer (CHT) problems that also involve advection. CHT with advection is a critical component of many important physical systems, for example thermal exchange along an ablating surface, and accurate robust treatment of these coupled systems has been a numerical challenge. The approach advocated here treats the governing temperature equations in different material domains using implicit time-stepping, while the interface coupling is explicit. The new approach, called the CHAMP scheme (Conjugate Heat transfer Advanced Multi-domain Partitioned), is based on a discretization of the interface coupling conditions using a generalized Robin (mixed) condition. The interface treatment combines ideas from optimized-Schwarz methods for domain-decomposition problems together with the interface jump conditions and additional compatibility jump conditions derived from the governing equations. The focus of the present work is primarily the development and analysis of a fourth-order accurate scheme, which is designed to be stable and accurate with minimal sub-iterations at each time step. Complicated geometrical domains are considered using overlapping grids, and results for a representative set of problems are presented. Time permitting, results coupling the new capability with high-order accurate incompressible flow solvers will also be discussed.

NS-ω-C Model for Fluid-Fluid Interaction Problems at High Reynolds Numbers

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November 8, 2021

Abstract

We consider a fluid-fluid interaction problem, where two flows are coupled through a nonlinear rigid lid condition, and one or both of these flows are at high Reynolds numbers. A method is proposed, that introduces the NS-ω-C turbulence model and combines it with a partitioning method called Geometric Averaging (GA) - so that the resulting model is efficiently decoupled, allows for the usage of preexisting solvers (e.g., air and water domain solvers), and is capable of resolving the flows at high Reynolds numbers. The NS-ω-C turbulence model, that we introduce in this report is a member of the newly proposed class of LES-C turbulence models, where a defect correction algorithm allows for the reduction of the modeling error. The resulting NS-ω-C-GA model is shown to be unconditionally stable and have optimal convergence properties. The model also allows for the non-filtered velocity in the interface terms; it has been shown recently that filtering the velocity in the interface terms could corrupt the quality of the model's solution.

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On the Stability of Interface Conditions for Ocean–Atmosphere Coupling

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Key Words: stability analysis, coupled system, partitioned algorithm, ocean-atmosphere

Numerical stability is of critical importance in general circulation models (GCM) because it affects the design of algorithms, time to solution, and computational costs associated with the simulations, which are very expensive in practice. Each component inside the coupled system is often associated with different time scales, posing a great challenge on time integration. In this work, our objective is to characterize the influence of different coupling strategies on the stability and accuracy of the fully coupled system.

We have analyzed the stability of different coupling strategies for multi-domain PDEs that arise in GCM. This study focuses on fully coupled ocean-atmosphere models that are needed to represent and understand their complicated interactions. In particular, we will discuss the stability of the coupled ocean-atmosphere models for various interface conditions such as Dirichlet-Neumann condition and bulk condition, which is unique to climate modelling. By analyzing a simplified model, we will show how the parameterization of the bulk condition and other physical parameters affect the coupling stability. By extending the analysis to a more realistic model that includes horizontal advection, we find that advection has a stabilizing effect in scenarios common to climate models when bulk interface condition and explicit flux coupling are used in tandem.

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Partitioned schemes with non-standard computational models. Part 1: Formulation*

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Key Words: *partitioned schemes, reduced order models, Lagrange multipliers*

Partitioned methods for multiphysics applications allow independent solution of computational models for each constituent component, thereby increasing computational efficiency of the simulation. This efficiency can be further increased by utilizing reduced order modeling (ROM) on select subdomains. In a series of two talks we present formulation and analysis of new partitioned schemes, which extend the approach in [1] and [2] to couplings of combinations of conventional Finite Element (FEM) and ROM sub-models. In Part 1 we present the formulation of a partitioned scheme for a model interface problem which couples a ROM with a conventional finite element method and extend the scheme to the case of coupling a ROM with a ROM. The proper orthogonal decomposition (POD) approach is implemented to construct a low-dimensional reduced basis on half the domain and solve the subdomain problem in terms of this basis using POD/Galerkin projection. The solutions on each half of the domain are coupled using a Lagrange multiplier representing the interface flux. The multiplier at the current time step can be expressed as an implicit function of the state solutions through a Schur complement. As a result, application of an explicit time integration scheme decouples the subdomain problems, allowing their independent solution for the next time step. We show numerical results that demonstrate the proposed method's efficacy in achieving both ROM-FEM and ROM-ROM coupling.

Disclaimer. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. SAND2021-14413 A.

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Space-time domain decomposition methods for the Stokes-Biot system

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Key Words: Domain Decomposition, Fluid-Poroelastic System

We consider decoupling iterative algorithms based on domain decomposition for the time-dependent Stokes-Biot model, in which different time steps can be used in the flow region and in the poroelastic medium. The coupled system is formulated as a space-time interface problem based on either physical interface conditions or equivalent Robin-Robin interface conditions. The interface problem is then solved by an iterative method which involves parallel solution of time-dependent homogeneous Stokes and Biot problems. Consequently, local discretization in both space and time can be used to efficiently handle multiphysics systems with discontinuous parameters. Numerical results with nonconforming time grids are presented to illustrate the performance of the proposed methods.

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The Schwarz alternating method for multiscale contact mechanics

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Key Words: Contact, Schwarz Alternating Method, Coupling, Multiscale

We introduce and evaluate numerically a fundamentally new approach to simulate mechanical contact based on the Schwarz alternating method. The new approach leverages our previous work in Schwarz multiscale coupling and addresses two well-known problems in computational simulation of contact: (1) the accuracy of the contact constraint enforcement, and (2) the multiple scales involved. Rather than introducing contact constraints into the variational form of the problem, as done in conventional contact techniques, the Schwarz alternating method decomposes the problem domain into two or more subdomains and prevents interpenetration by applying transmission (boundary) conditions in an iterative and alternating fashion on the subdomain boundaries. The Schwarz alternating method has a number of desirable qualities, including its ability to use different element topologies and time integrators in different subdomains. We demonstrate herein that these advantageous properties carry over to the contact variant of the method.

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The Schwarz alternating method for ROM-FOM coupling

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Key Words: Schwarz alternating method, domain decomposition, projection-based reduced order model (ROM), heterogeneous coupling

Although projection-based model order reduction is a promising approach for enabling real-time and multi-query analyses, reduced order models (ROMs) have been known suffer from a lack of robustness, stability and accuracy, especially in the predictive regime. This talk describes a new methodology for improving the predictivity of projection-based ROMs by coupling these models conventional full order models (FOMs) using the Schwarz alternating method. The Schwarz alternating method [1] is based on the simple idea that if the solution to a partial differential equation (PDE) is known in two or more regularly-shaped domains comprising a more complex domain, these local solutions can be used to iteratively build a solution on the more complex domain. Leveraging recent work that adapted the Schwarz alternating method to enable consistent and concurrent multi-scale coupling of finite element FOMs in solid mechanics [2, 3], we present a new extension of the Schwarz formulation that enables ROM-FOM coupling. The new approach is based on the following ingredients: (i) a decomposition of the physical domain of interest into two or more overlapping subdomains, (ii) the construction of either a FOM or a projection-based ROM in each of the subdomains, (iii) the definition of appropriate transmission boundary conditions (BCs) which will propagate information between the overlapping subdomains, and (iv) the introduction of a Schwarz iteration process in which the ROM and FOM solutions on each subdomain are successively updated (to convergence) in an iterative and alternating fashion, with information between subdomains propagating through the transmission BCs. After describing the method's formulation and theoretical properties, we evaluate its performance on several numerical examples from the field of solid mechanics. Specifically, we demonstrate that the method is capable of producing a more accurate solution than the classical single-domain Proper Orthogonal Decomposition (POD)/Galerkin ROM approach, while still achieving a computational savings with respect to a typical FOM discretization.

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Contact Force Parameter Sensitivity in Stirred Mills

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Key Words: *Discrete element method, Parameter sensitivity, Parameter estimation*

Determining the correct pairwise parameters in a Discrete Element Method (DEM) contact force model is a non-trivial undertaking. Difficulty in parameter estimation is in part due to correlation between parameters and observed system responses[1]. Additional considerations include the process conditions, for instance, if a system is in a friction-driven regime then any contributions from non-friction parameters in the model are masked to an extent, which can hinder estimation.

This work analyses DEM model parameter sensitivities following the methodology outlined by Yan, et al.[1], applied to a stirred milling system instead of a cylinder with an orifice; thus, energy is imparted into the system via the geometry and not solely gravity. Further, the process settings of the stirred milled are varied. This is to both identify the difference between particle-particle and particle-geometry term sensitivities and to link differing process regimes with changes in parameter sensitivity. The methodology considers 3 increasingly detailed levels of statistical analysis:

1. Analysis of fitting parameters for empirical model.
2. Principal Component Analysis (PCA) on simplified contact model derivatives.
3. Analysis of sensitivity matrix constructed from full contact model derivatives.

In this work, the Hertz-Mindlin[2] and Constant Directional Torque[3] (CDT) contact models are used to describe collisions of the milling grinding media for a dry operation simulation. Varied parameters are the coefficient of restitution, sliding and rolling friction. Additionally, the analysis is applied to 4 varied process settings corresponding to different filling levels and attritor speeds. The variable used during this analysis is the grinding media Root-Mean Square (RMS) velocity, a relevant variable within milling[2]. The analysis for each level showed that:

1. A fully packed system showed little variance in parameter dependency, the opposite was true when the filling level was reduced.
2. The equation of mass terms varied more with fill level than for moment of inertia.
3. Particle-geometry terms had greater impact than particle-particle terms. The equation of mass is dominated by coefficient of restitution and moment of inertia by rolling friction.

Thus, the process conditions chosen can have an impact on the present sensitivities of the utilised DEM model, and care should be taken to determine the regimes present that are within the modelling scope, with estimation data taken from each regime. Hence, the estimation will improve as the parameters exhibit noticeable variance that can be identified by a minimisation routine.

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Coupled PFEM-DEM-FEM Model of a Stirred Media Mill

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Key Words: Particle Finite Element Method, Discrete Element Method, Coupled Models, Stirred Media Mill

In the mining industry, comminution is the single most energy-intensive process accounting to approximately 4 % of the global produced electric energy [1] and as much as 50 % of the electric energy consumed in a mine can be attributed to comminution [2]. Stirred media mills have a high energy efficiency compared to other commonly used mills, such as ball mills. Modelling a wet comminution process is challenging since it requires consideration of the complex multi-physics in the mill. It requires the simultaneous treatment of feed material, grinding fluid and media, and rotating internal agitator elements. In this study, a model of a pilot vertical stirred media mill with a nominal power of 7.5 kW is developed. The model utilizes a particle-based coupled solver approach, where a Particle Finite Element Method (PFEM) [3] model is coupled with a Discrete Element Method (DEM) [4] model and a Finite Element Method (FEM) model. PFEM is used to model the grinding fluid, DEM to model the grinding media and FEM to model the mill structure, i.e., the agitator elements. The models are coupled by a loose (or weak) two-way coupling strategy. A Reynolds number dependent drag coefficient is used in the PFEM-DEM coupling and the grinding fluid is modeled as a non-Newtonian, shear thinning fluid. By the coupled PFEM-DEM-FEM models the complex dynamics inside the stirred media mill are predicted. The model is used to quantify the power consumption, wear distribution on agitator elements, inter-particle collisions and grinding media and fluid dynamics in the stirred media mill. The model is validated against experimental measurements of power consumption on a pilot mill with good agreement.

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DEMvironment: A Workflow Environment for Advanced DEM Parameter Calibration

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Key Words: *Calibration, Discrete Element Method, Automated Workflows, Granular Materials*

Although the discrete element method (DEM) is widely used to study granular materials in diverse scientific and engineering applications, the choice of the DEM input parameters is still a challenge. On the one hand, it is often difficult to measure individual particle or particle-particle interaction parameters. On the other hand, due to key simplifications made in existing contact models or the shape and deformation of particles, these measured properties would not reproduce the actual bulk behavior with sufficient accuracy. In addition, advanced closure models for the DEM have been developed, e.g., contact force closures for very densely packed granular materials [1], [2].

Following any of the existing calibration methods, i.e., either the direct bulk calibration [3] or response surface generation methodology [4], demands (i) conducting multiple simulations and (ii) a comparison with experimental or relational data[5]. In our newly developed tool "DEMvironmnet", Orange3 [6] workflows and Python modules are integrated to set up, manipulate and run calibration workflows. The Aspherix® Calibration software is used as the numerical heart of our calibration workflow, realizing a comfortable direct bulk calibration. Moreover, DEMvironment provides a graphical interface to demonstrate the flow of data and visualize the data handling strategy. Our tool follows four main steps in a calibration workflow: (i) data handling, (ii) calibration, (iii) data storage, and (iv) validation. Step (i) assists the user in input data preparation, processing output data from simulations, and interactions with a central database. Step (ii) performs the actual calibration of parameters, and steps (iii) and (iv) help in storing and validating a calibrated DEM-based simulation.

DEMvironment expedites the often demanding calibration procedure, and facilitates the reusability of valuable data from experimental studies of granular matter. In our presentation, this tool is explained in greater detail, as well as providing application use cases. We close our presentation by highlighting how DEMvironment could be used to calibrate parameters of an advanced multi-contact force closure for highly compacted granular materials [2].

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Digital Twins of Widely-Used Powder Characterisation Tools

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Key Words: DEM, Particle-Properties, Calibration

Discrete-Element-Method (DEM) simulations are a valuable tool for research and industry to model experiments or industrial processes involving particulate media. These simulations can predict the anything from the strength of a con- crete block to the damping efficiency of granular dampers, as well as helping us better understand complex phenomena such as the granular Leidenfrost effect or the Brazil-Nut Effect.

While they are capable of quantitatively reproducing the dynamics of real- world systems, their validity depends strongly on the calibration of the simula- tion – i.e. the implementation of exact particle properties such as the Coefficient of Restitution or the Young's Modulus. These properties usually are defined by the material and shape of the used particles which must typically be determined through multiple, complex and highly labour-intensive experiments. Indeed, this calibration process can be the most time consuming part in modelling of a scientific or industrial system – a significant problem in industry in particular, where time efficiency is paramount.

To address this issue, we have developed a series of open source DEM Digital Twins of widely used powder characterisation tools, namely the FT4 Powder Rheometer with its dynamic and shear cell methodology, the Schulze shear cell and the GranuTools GranuDrum and GranuHeap. Each of our Digital Twins extracts realistic data – as each real device would – which can be used to fine tune powder properties in your simulation. The open source package features a coupling to the LIGGGHTS simulation engine, advanced mesh control to allow the quick change between mesh movements and specialised image extraction techniques from DEM data. We show a example application of the digital twin on a common calibration problem using coarse grained particles.

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Discrete Element Simulations from two-dimensions with polygons to three dimensions with rods

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Key Words: Discrete element method, Polygonal shapes, Polyhedral shapes, Schneebeli Material

Discrete Element (DEM) simulations in two dimensions reproduce characteristic features of three-dimensional experiments as long as the system is a cross section with respect to a symmetry. Examples are central pressure "dips" for heaps built in a wedge - but not in a layered - sequence [1] as well as characteristics of stress-strain curves (linear regime for small strains, maximum for non-spherical particles, lack of maximum for spherical particles [2], higher strength for non-convex than for convex particles [3]). Experimentally, quasi-two dimensional systems have been realized by "Schneebeli-Material", parallel rods of even cross-section, which have been used for shear- and failure experiments for a long time. However, it is far from clear how much two-dimensional simulation results will match experimental data in three dimensions, as there is a crucial difference in the dynamics of two and three dimensions: Straight lines "nearly always" intersect in 2D, so that vectors of strong forces will meet in the force networks and can so destroy the stability of the assembly. Skewed lines in three dimensions do not intersect, and so vectors of strong forces will not meet. As a consequence, the mechanical stability of 3D assemblies (mostly, but not perfectly parallel rods) should be higher than that of polygons in 2D for the same cross sections. In this research, we investigate the stress-strain diagrams with DEM-simulations for rods with polygonal cross sections in three dimensions[4] and of polygons in two dimensions for two-axial compression.

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EXPERIMENTAL VALIDATION OF THE LINEARISED $\mu(I)$-RHEOLOGY APPLIED TO ROTATING DRUM FLOWS SPANNING ROLLING-TO-FULLY CASCADING FLOWS

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Key Words: *PEPT, tumbling mills, granular rheology, coarse-graining*

Depth-integrated formulations underpinned by the linearised $\mu(I)$-rheology [1,2] and the *shallow flow approximation* [3] offer useful qualitative insights into rotating drum flows operated in regimes spanning straight and minimally curved free surfaces characterised by Froude numbers less than 0.3. Beyond these regimes (Fr > 0.3) the solution fails to recover a realistic bed geometry and flow field. To extend the theory to Fr > 0.3 we relax the shallow flow approximation and apply corrections to the velocity field before reconstituting the mass, momentum and energy balances. Positron Emission Particle Tracking (PEPT) experiments of a 476 mm diameter drum (length of 200 mm) filled to 50 percent of drum volume with 3 mm glass beads was used to validate the updated theory. To ensure equitable comparison, the PEPT data is coarse grained [4] into voxels of dimensions 2.5 times the particle diameter. Using the same averaging window, the theory is tuned against the PEPT solution. Quantitative comparisons of the velocity field, bed geometry (free surface and basal interface), energy dynamics and principle stresses show statistical agreement for all drum speeds investigated. The tuned theoretical parameters—slope of the linearised rheology χ, dilated fill fraction ζ, and bed repose angle α—are then correlated with drum speed. The aforementioned procedure allows for full flow field prediction of a given granular material flowing in rotating drums operated at Fr > 0.3.

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Particle Flow and Heat Transfer in Pharmaceutical Operations

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Key Words: *Granular Flows, Discrete Element Method, Heat Transfer, Drying, Conduction.*

Processing of particulates plays an important role in a wide variety of industries, including the pharmaceutical industry, the bulk chemical industry, and the food industry, to name a few [1]. Yet, despite the ubiquity of particulate systems, a strong fundamental understanding of their behavior is lacking. We have focused on heat transfer in granular materials in order to better understand the drying of particulates. Drying is an important manufacturing step in the production of active pharmaceutical ingredients (APIs) [2]. Several approaches exist to carry out the drying procedure, but a common method used by the pharmaceutical industry is agitated drying. During the process, a wet bed of API is heated in a jacketed cylindrical vessel while being mixed by a rotating impeller until the moisture content is reduced to a desired level. This geometry can be simplified as a vertical cylindrical vessel in which wet particles rest at the bottom of the unit. Heat is typically supplied via conduction through a heated jacket around the wall of the vessel while an impeller, which can also be heated, mixes the particles to help improve the distribution of heat and promote evaporation throughout the bed. This geometry offers several notable benefits in terms of design, such as its high thermal efficiency, low cost of operation, and environmental advantages. Another significant advantage is that it can be equipped with a filter and thereby enable API filtration to be carried out in the same unit prior to drying. This reduces the potential for product loss that can occur when transferring material to a different equipment and decreases the risk for worker exposure to potent and possibly toxic materials.

The complexity of the process stems from the fact that heat transfer, mass transfer, and changes in physicochemical properties can occur simultaneously throughout drying. Complications often plague the procedure, including issues such as lengthy drying times, over-drying, nonuniform drying, agglomeration, attrition, and form changes. These circumstances make agitated drying a complicated process to understand and control. When considering scale up, these challenges are coupled with the difficulties typically associated with transferring knowledge from lab scale to pilot or manufacturing scale. As a result, it can be difficult to design an appropriate drying protocol that optimizes heat transfer and can be translated from scale to scale while minimizing the risk for adverse conditions. In this work, we decouple the problem and focus on studying the heat transfer aspect of agitated drying. More specifically, we investigate the influence of process and material parameters on heat transfer in an agitated bed of particles. Our approach consists of employing a combination of experiments and discrete element method (DEM) modeling techniques to analyze how heat transfer scales with flow, mixing and bed parameters. We have carried out a design of experiments and computed heating times as well as heat transfer coefficients and temperature distributions for the different conditions. We find that scaling influences the flow and compressibility of the bed and therefore creates a balance between conduction and granular convection as the dominant mode of heat transfer.

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RADAR PARTICLE TRACKING AS A CALIBRATION TOOL FOR MODELING PARTICULATE MATERIALS

TRACK NUMBER 1000

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Key words: Granular, particulate, calibration, validation, particle tracking, radar

ABSTRACT

Through continuous development in the past century, radar (radio detection and ranging system) technology has advanced into a versatile approach being widely used in various disciplines, from conventional moving target indicator radar via ground penetration radar to synthetic aperture radar for space exploration and satellite imaging [1]. In particular, the development of semiconductor industries enables the integration of a whole radar system on a silicone chip, thus dramatically facilitates the application of radar systems in non-destructive testing (NDT) as well as in consumer products (e.g., smartphone) to enhance human-machine interactions.

Here, we describe the possibility of using radar particle tracking technique as an alternative approach to track projectile motion inside granular media. After a brief description of the advantages and disadvantages of the small scaled multi-static continuous wave radar system, the implementation of this approach in monitoring granular drag will be presented [2]. Subsequently, we focus on the implementation of this approach in the calibration of DEM simulations for a better understanding of the influence of gravity on granular drag [3]. Eventually, a brief outlook into the future of radar systems in verifying large scale computer simulations will be provided to trigger further discussions and potential applications.

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Regional Heat Transfer in Coffee Roasters Determined via PEPT Validated DEM & CFD-DEM Simulations of Coffee Bean Particle Motion

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Key Words: *Coffee Roasting, Heat and Mass Transfer, Simulation, PEPT, CFD-DEM, DEM.*

Understanding physicochemical coffee bean development during roasting is integral to unlocking key flavour and aroma characteristics, as well as improving process efficiencies and translating products from one roaster to another. Simulation of roasting time-temperature profiles currently rely on semi-empirical heat and mass transfer models. These empirical models alone cannot quantify the variation of air-to-bean heat transfer induced by particle flow patterns. By identifying coffee bean particle motion within a roaster, particle dynamics can be coupled with heat and mass transfer models to improve both the accuracy and robustness of time-temperature profile simulations.

Experimental flow studies of coffee beans have been performed using Positron Emission Particle Tracking (PEPT) to capture particle motion within two roaster designs: (i) rotating drum, (ii) spouted bed. These experimental data were then used to rigorously calibrate (i) a DEM simulation of the rotating drum, (ii) a CFD-DEM simulation of the spouted bed, thus quantitatively acquiring the complex dynamics of aspherical particle motion in process equipment.

Determination of occupancy and velocity profiles revealed two distinct regions for both systems (i) a dense bean bed of high occupancy with low particle velocity (ii) a dilute freeboard of lower occupancy with higher particle velocity. By examining the boundaries of the delineated bean bed and freeboard, and how they transform due to changes in coffee density and applied process parameters, heat and mass transfer properties of the system can be inferred. Established empirical properties can thus be integrated with heat and mass transfer models to indicate regional heat transfer contributions.

PEPT validated CFD-DEM/DEM simulations provide fundamental knowledge of system dynamics that have been used to develop more accurate and robust physics-driven models of coffee roasting. Commercial implementation of these models thus has the potential to virtualise the roasting process and overcome trial and error approaches to product and process development.

Statistical comparison of coarse-grained kinematic fields derived from Postron Emission Particle Tracking (PEPT) Experiments and Discrete Element Method (DEM) simulations in rotating drums

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Key Words: *PEPT, DEM, tumbling mills, granular rheology, coarse-graining*

In the absence of a universally accepted, fundamental theory that describes dense granular flows, researchers must resort to dimensional analysis to understand the drivers of the system. Leading theories on granular flow [1,2] are underpinned by dynamic properties like the shear rate and granular temperature; the shear rate is vital to quantify the slurry viscosity—a key parameter controlling slurry transport in rotating drums, for example. Such properties are readily derived from numerical DEM simulations which are capable of producing discrete, microscale data at a timestep of 10^{-6}s. We argue that one can trust this dynamic data if-and-only-if it is validated against experimental measurement. In this regard PEPT, a Lagrangian, nuclear imaging technique, is capable of producing full 3D kinematic data (solids fraction, velocity) at ~10^{-3}s. To this end, we perform PEPT measurements and DEM simulations of three and five millimetre monosize glass beads in a 300mm, 30% filled rotating drum at high Froude regimes. The resultant PEPT kinematic data is coarse-grained [3] to produce continuum kinematic fields; this process requires tedious calibration, in an iterative sense, by choosing the optimal smoothing radius such that a continuous profile is generated. These PEPT fields (solids fraction, velocity maps) are then subjected to statistical comparison against DEM-based continuum fields. The shear rates are subsequently evaluated by applying approaches proposed by [3] and [4] to the now validated PEPT and DEM velocity fields. The latter approach [4] is more favourable because it does not require tuning of any parameters, i.e., smoothing radii. In the event of poorly sampled data, one is better off using the [3] model which incorporates neighbouring cell data to produce a smooth continuum description. Statistical comparison of continuum data at in high Froude regimes is seminal and as such, this work offers useful insights into the coarse graining of Lagrangian kinematic data to produce continuum fields.

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A simple Augmented Lagrangian and arc-length methods coupling for simulation of shells and trusses with equality restrictions.

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1. Abstract

This paper presents a simplified implementation of the arc-length method for computing the equilibrium paths of nonlinear structural mechanics problems with equality restrictions imposed by the augmented lagrangean method. In this work, the predictor is based on extrapolation from two previously converged load steps and the lagrangian multiplier is updated in the usual way, in relation to the penalty parameter and the penetration. The extrapolation being a simple linear relation renders a simple method of update that additionally serves as way of identifying the forward movement along the equilibrium path, without the need of any complex technique commonly employed for explicit tracking. The capability of the algorithm to correctly describe the equilibrium path is verified in static structural mechanics problems through benchmarks from the literature. The results indicate that the algorithm is fully capable of reproducing all of the verified examples.

Development of 3D visualization system from 2D Plane Figures

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Key Words: *Image recognition, Spatial cognition, AI, AR, OpenCV*

Contents using AR (Augmented Reality) and VR (Virtual Reality) are expected to be useful in various fields including scenes of broadcasting and education. The combination of visual information and reality increases volume of information and enhances the human capability. In particular, the introduction of ICT into school education have been active and the value is drawing increasing attention over the recent years. Under the circumstances, we considered a system that supports learning by assisting spatial ability with AR[1].

Spatial ability is the capacity to recognize relations or appearances of objects in a 3D space. This ability depends on individual in its accuracy or speed of understanding. Learning methods are changing on the stages of development of learners. For examples, during childhood, putting the blocks together or making solid model physically are performed to acquire spatial ability, but the middle and high school use only texts generally. Learning using real objects like blocks help to understand 3D intuitively because it can link real movements with vision. However, learning using only text requires a higher level of spatial ability.

In this paper, we developed an application to reduce the effects of differences in spatial cognitive ability in learning by using AR to visualize 2D figures in 3D and help learners to acquire spatial ability and grasp the image of the plane-to-three-dimensional transformation. The system generates 3D data automatically based on the features of a 2D plan view and then displays it as AR. The feature point extraction and coordinate recognition are performed by the OpenCV library and figure identification is performed by machine learning technology. Based on these results, 3D model is generated and displayed as AR on a web browser by AR.js.

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Development of Huge-Scale Microwave analysis software: ADVENTURE_Fullwave

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Key Words: *Microwave Analysis, E-Method, Parallelized Finite Element Method, Domain Decomposition Method, ADVENTURE_Fullwave.*

Electromagnetic field analysis based on a numerical analysis method, such as the finite element method, has become widespread [1] due to recent improvements in computer performance and numerical calculation technology. In the case of accurately reproducing an analysis model of complicated shape, it is necessary to use many small the elements. In the case of analyzing the state of electromagnetic waves propagation in a wide range, a wide analysis domain is examined. Furthermore, to perform a high-accuracy analysis, it is necessary to model the analysis domain with a sufficiently small element for the wave-length, and, in this case, the number of elements also increases. Increasing the number of elements increases the scale of the problem. Therefore, a method that can calculate large-scale problems has come to be demanded. Moreover, large-scale problems must be solved with high accuracy.

In this presentation, a huge-scale microwave analysis software based on an iterative domain decomposition method is explained that is named ADVENTURE_Fullwave [2]. A stationary vector wave equation for the high-frequency electromagnetic field analyses is solved taking an electric field as an unknown function. Then, to solve subdomain problems by the direct method, the direct method based on the LDL^T decomposition method is introduced in subdomains [3][4][5]. The simplified Berenger's PML is introduced which these eight corners are given the average value of all PML's layers.

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Effect of Metabolic Heat Generation, Blood Perfusion and Environment Temperature on the Body Temperature-an Approach of Finite Element Simulation

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Key Words: Bio-heat transfer; whole body model; tissue temperature; finite element and ADVENTURE_Thermal.

Metabolic heat generation, blood perfusion and surrounding conditions have effect on the human body temperature. Considering these effects, the natural thermoregulatory system maintains the comfortable body core temperature.

The aim of this study is to investigate the effect of metabolic heat generation, blood perfusion rate and ambient temperature on the body temperature during different physical activities. Penne's bio-heat equation is being widely used for the simulation of the skin burn [1] and temperature controlled thermal ablation [2]. For the current investigation, three dimensional finite element model of bio-heat equation has been developed and added in the ADVENTURE_Thermal [3].

The heat transfer analysis was performed in the three dimensional skin and simple human body model using the developed system. The skin temperature was investigated with a hot disk and hot coffee in touch separately. A simple human whole body model has been developed and the effect of the mentioned physiological parameters on the body temperature was measured.

The numerical results depict that blood perfusion rate acts as a heat sink when the extra metabolic heat is generated. The body temperature variates with different metabolic heat generation and ambient temperature during cooking, walking and running at different velocities. The developed model and the system will help investigate the body temperature in the clinical treatments.

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Efficient Implementation
of Skyline Solver for Many Core and GPU Environment

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ADVENTURE AutoLinAS (pronounced as 'O-to-li-na-shi') is a linear algebraic solver library, dedicated for simulation-based research and development. It is designed for the simulation users to develop their own solvers. Currently, the library is used among many researchers and simulation users, mainly in universities and national research centers. Its functionalities and supported platforms are explained. AutoLinAS applications of various kinds of simulation methods are demonstrated also.

Implementations of the library for various kinds of high performance computing platforms, such as Intel x86, Intel Xeon, AMD EPYC and Fujitsu PRIMEHPC FX-1000/Fugaku, as well as NVIDIA GPU, are available. Each of them is highly tuned for the underlying hardware architecture.

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Fast Electrostatic Field Analysis with Unstructured Numerical Human Body Model Using Parallel Geometric Multigrid Method

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Key Words: *Marching Cube, Mesh Smoothing, Geometric Multigrid Method, Electrostatic analysis*

In electrostatic field analysis using a numerical human body model constructed with voxels, the electric field strength is overestimated near the staircase boundary of different materials (called staircasing errors)[1]. To reduce these staircasing errors, mesh smoothing based on the marching cubes method is developed and applied to the numerical human body model [2]. The extended marching cube method is proposed in this research, which can perform mesh smoothing of three kinds of boundaries, and most of the 90-degree angle points of the boundary of different materials in the numerical human body model can be smoothed.
In addition, in order to cope with the increase of computation time due to the increase of DOFs by mesh smoothing, the geometric multigrid method [3] for unstructured grids is applied to the numerical human whole-body model, and the computation time per subdivision is compared with that of the CG method solver with preprocessing. As a result, it is found that the geometric multigrid method can reduce the increase of computation time per subdivision compared with the CG method with preprocessing. In terms of computation time, the geometric multigrid method achieves a maximum computation time of about 1/20 of that of ILU-CG for voxel models and about 1/15 for smoothing models.

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Motion Feature Analysis of Noh Dance using ANN based Motion Capture Technology

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Key Words: *Noh, Traditional dance, Motion analysis, Motion capturing*

Noh is one of the most representative traditional art forms in Japan. Since the 14th century, *Noh* has continuously been inherited for more than 700 years. *Noh* also has been registered as an intangible cultural heritage by UNESCO. A previous study showed that *Noh* movements can be used to keep elderly people's health. Today *Noh* is not only for people to enjoy in the theatre, but *Noh* is also useful for health promotion. The benefits are both on maintaining health and beautiful standing posture.

Hakobi (Sliding walk) is one basic movement pattern of walking in *Noh*, which refers to walking with the feet sliding on the floor slowly. The sliding walk is very different from the walking in daily life and can be used to exercise the psoas major muscle. In this research, we analyzed the features of sliding walk. We also compared the motion of sliding walk and walking.

For motion tracking techniques, the traditional marker-based motion capture system is constrained by the utilization of the environment. For example, a stage costume is important for any dance performance, but markers are not suited for a dancer's stage costume. Therefore, we use artificial neural network-based motion capture technology to recognize human pose without markers. In this research, OpenPose[1], one of the most popular open-source libraries, is used for pose estimation from video images.

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Performance evaluation of parallel wave-sound analysis software: ADVENTURE_Sound

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Key Words: *Wave-sound Analysis, Parallelized Finite Element Method, Domain Decomposition Method, ADVENTURE_Sound.*

A wave-sound analysis based on a numerical analysis method, such as the fi-nite element method, has become widespread due to recent improvements in computer performance and numerical calculation technology. In the case of accurately reproducing an analysis model of complicated shape, it is necessary to use many small the elements. In the case of analyzing the state of wave-sound propagation in a wide range, a wide analysis domain is examined. Furthermore, to perform a high-accuracy analysis, it is necessary to model the analysis domain with a sufficiently small element for the wavelength, and, in this case, the number of elements also increases. Increasing the number of elements increases the scale of the problem. Therefore, a method that can cal-culate large-scale problems has come to be demanded. Moreover, large-scale problems must be solved with high accuracy. In the presentation, ADVENTURE_Sound is introduced, and some numerical result in the performance evaluation for the parallel computing environment: Work-station Cluster is shown.
In this presentation, a performance evaluation of the paralell wave-sound analysis software based on an iterative domain decomposition method is explained that is named ADVENTURE_Sound [1]. A wave-equation for the wave-sound analyses is solved taking a speed potential as an unknown function. In this software, an iterative domain decomposition method is employed as a parallel technique. To solve subdomain problems by the direct method, the direct method based on the LDL^T decomposition method is introduced [2][3][4]. In this paper, some numerical results are discussed in the view point of a performance for parallel computing environments.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Uncertainty Quantification Using Non-Intrusive Polynomial Chaos Method for Large-Scale Electromagnetic Wave Analysis

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Key Words: Uncertainty Quantification, Non-Intrusive Method, Monte Carlo Simulation, Large-Scale Analysis, Parallelized Finite Element Analysis

In numerical analyses of physical phenomena, it is necessary to analyze stochastically if geometries, material properties, and boundary conditions of the analysis objects have uncertainties. The field of evaluating the influence of uncertainties of parameters in simulations is called Uncertainty Quantification or UQ in short. UQ has attracted more attention in recent years because it can be used for reliability evaluation, optimization, and safety evaluation in the design of systems and devices.

One of the most widely used methods for UQ is the Monte Carlo simulation. The method evaluates probability distributions of output parameters by generating random numbers which follow a specific probability distribution of input parameters and then calculating the output value for each random number. While a deterministic simulator can be utilized as a black box, the application of the method is limited to small-scale analysis because of the need for a quite large number of samples to achieve good approximation. Therefore, Spectral Stochastic Finite Element Method [1] was devised by Ghanem and Spanos. In this method, input and output random fields are discretized by spectral expansions in probability space, and the probability distribution of the output can be evaluated by a single matrix calculation. Although having high computational efficiency, it takes much labor to modify existing codes.

The purpose of this paper is to quantify uncertainties in the large-scale analysis of physical phenomena using a non-intrusive method, which has the advantages of both of the above two methods. The non-intrusive method has reusability of existing codes and high computational efficiency, and therefore it is easy to apply to large-scale problems. In the present study, we integrated the non-intrusive method with the ADVENTURE [2], a deterministic simulator based on a parallelized finite element method, to perform a large-scale electromagnetic wave analysis with uncertainties. Specifically, we stochastically evaluated the electromagnetic fields in the human body whose permittivity and conductivity have uncertainties.

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Multilevel and domain decomposition methods for solving large scale phase-field fracture simulations

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Key Words: Phase-field fracture, Non-convex optimization, Multilevel and domain decomposition methods

One of the state-of-the-art strategies for predicting crack propagation, nucleation, and interaction is the phase-field approach. In this approach, a damage variable is introduced to characterize the material state from intact to fully broken. Although the phase-field approach is a robust tool for predicting crack propagation, it gives rise to strongly nonlinear coupled systems of nonlinear equations that have to be solved at each time step. This is computationally challenging due to the non-convexity of underlying energy functional, a large number of degrees of freedom, and the severe ill-conditioning caused by the local changes in the damage variable.

In this work, we propose to solve the arising nonlinear problems efficiently using multilevel [2] and domain decomposition [1] methods. The proposed methods are designed to solve the arising non-linear problems in a monolithic manner by taking advantage of the underlying structure of the coupled problem. In particular, we discuss different techniques to construct a hierarchy of suitable subspaces, related to different levels or subdomains. In the multilevel settings, we employ novel level-dependent objective functions, that combine a fine-level description of the crack paths with the coarse level discretization. For the domain decomposition, we take advantage of partitioning the degrees of freedom into two sets, related to the displacement and the phase-field. Eventually, we combine both, multilevel and domain decomposition, techniques with the trust-region globalization strategy in order to ensure global convergence.

We will demonstrate the convergence behavior of the proposed multilevel and domain decomposition methods using several benchmark problems. A comparison with the widely-used alternate minimization method will be presented, showing a significant reduction in the number of iterations and the execution time. In the end, we will also illustrate the strong and weak scaling properties of the overall simulation framework.

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Numerical modeling of injection-induced slip and propagation of fractures in poroelastic media

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Key Words: *Mixed-dimensional model; Mixed-mode fracture propagation; Contact mechanics; Coupling discretization methods; Hydraulic stimulation; Poroelasticity; Multiscale simulation; Open-source software.*

Fractures play an essential role in the enhancement of geothermal reservoirs through hydraulic stimulation, where the overall reservoir permeability can be enhanced both by slip and dilation of existing fractures and by fracture propagation. We present a mathematical model and numerical strategy to investigate the interaction between fluid flow, deformation, fracture shearing, and fracture propagation during low-pressure fluid injection. Deformation and fluid flow are represented based on a mixed-dimensional model, considering fractures as co-dimension one objects in the domain. The matrix surrounding the fractures is poroelastic, and a contact mechanics model govern the deformation of existing fractures. Mixed-mode fracture propagation is modelled by the maximum tangential stress criterion.

The solution approach is based on a multiscale strategy, expanding on the work by Dang-Trung et al. [1]. In the macroscale model, flow in and poroelastic deformation of the matrix are coupled with the flow in the fractures and fracture contact mechanics [2], allowing fractures to frictionally slide. Fracture propagation is handled at the microscale. Simulations show how the shearing of a fracture due to fluid injection is linked to fracture propagation, including cases with hydraulically and mechanically interacting fractures.

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Analytic Solutions of 2-D Transient Heat Conduction Problems by the Symplectic Superposition Method

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Key Words: *Heat Conduction, Heat Source, Symplectic Superposition Method, Analytic Solution*

In view of the important role in providing benchmarks and rapid parametric analyses for preliminary designs, analytic solutions gain permanent interest for heat conduction problems. In this study, the 2-D transient heat conduction problems with or without heat sources in a rectangular domain under different combinations of temperature and heat flux boundary conditions are studied by a novel symplectic superposition method (SSM) [1-4]. The solution process is within the Hamiltonian system framework such that the mathematical procedures in the symplectic space are implemented, which provides an exceptional direct rigorous derivation without any assumptions or predetermination of the solution forms compared with the conventional inverse/semi-inverse methods. The distinctive advantage of the SSM offers an access to new analytic heat conduction solutions. The accuracy of the SSM is confirmed by comprehensive transient heat conduction results, including both numerical and plotted temperatures, as validated by the finite element method. This study is the first one on extending the SSM to heat conduction problems, which may pave the way to more benchmark analytic solutions in the field.

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Development of 3D Fiber Computational Grains for the Micromechanical Modeling of Fiber-Reinforced Composites

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Key Words: *Computational Grains, Fiber Composites, Papkovich-Neuber solutions; parallel computation.*

In this study, 3D fiber computational grains (CGs) are developed for the micromechanical modelling of fiber-reinforced composites. The microstructure of a fiber composite can be divided into several CGs, each of which contains a long fiber. And a compatible displacement field is assumed at the outer-boundary and the fiber-matrix interface in each CG. Trefftz trial displacement fields in each element are expressed in terms of Papkovich-Neuber solutions, by employing cylindrical harmonics as Papkovich-Neuber potentials. A new scaling method for the cylindrical harmonics is proposed to avoid solving ill-conditioned equations. And the element stiffness matrix of each CG is derived by a new kind of multi-field boundary variational principle. By several numerical examples, we demonstrate that the developed CG is an efficient and accurate numerical method for computing the equivalent material properties and the micro-scale stress distribution of fiber composites. Moreover, the computational efficiency of the CG is enhanced with the use of the parallel computation. In this way, a RVE with 2500 fibers can be simulated within 10 hours on an 8-core laptop.

New Straightforward Benchmark Solutions for Bending and Free Vibration Solutions of Clamped Anisotropic Rectangular Thin Plates

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Key Words: *Anisotropic Plate, Bending, Vibration, Benchmark Solution, Finite Integral Transform*

This study presents new straightforward benchmark solutions for bending and free vibration of clamped anisotropic rectangular thin plates by a double finite integral transform method [1]. Being different from the previous studies that took pure trigonometric functions as the integral kernels [2–6], the exponential functions are adopted, and the unknowns to be determined are constituted after the integral transform, which overcomes the difficulty in solving the governing higher-order partial differential equations with odd derivatives with respect to both the in-plane coordinate variables, thus goes beyond the limit of conventional finite integral transforms that are only applicable to isotropic or orthotropic plates. The present study provides an easy-to-implement approach for similar complex problems, extending the scope of finite integral transforms with applications to plate problems. The validity of the method and accuracy of the new solutions that can serve as benchmarks are well confirmed by satisfactory comparison with the numerical solutions.

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Symplectic Superposition Method for Analytic Solutions to Plate and Shell Problems

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Key Words: *Symplectic superposition method, Plate, Shell, Analytic solution*

Plates and shells are widely used in various fields such as civil engineering, mechanical engineering, ocean engineering, aeronautics and astronautics. Solution for bending, vibration and buckling of plates and shells has been one of the important research topics in engineering. However, it is hard to obtain the analytic solutions to most of these problems till now due to the mathematical challenge. Using an up-to-date symplectic superposition method, we obtain the analytic solutions of plates and shells with various boundary conditions, by which the ability of the method to yield solutions via step-by-step derivations from the governing equations without predetermining any forms of solutions is demonstrated. The essential difference between the current method and the other ones is that the solution procedure is conducted in the symplectic space rather than in the classical Euclidean space. This extends the scope of application of eigen expansion, and paves the way for more analytic solutions of similar problems. The application of the method to novel stretchable electronics is also reported, which provides a theoretical basis for fracture-safe design of stretchable electronics.

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An industry-relevant implicit LES via spectral/hp element methods

Gianmarco Mengaldo, David Moxey, Michael Turner, Rodrigo C Moura, Ayad Jassim, Mark Taylor, Joaquim Peiro, Spencer J Sherwin

We present the successful deployment of high-fidelity Large-Eddy Simulation (LES) technologies based on spectral/hp element methods to a real automotive car, namely the Elemental Rp1 model [1]. The simulation presents the common challenges of an industry-relevant simulation, namely high Reynolds number and complex geometry. To the best of the authors' knowledge, this simulation represents the first fifth-order accurate transient LES of an entire real car geometry. Moreover, this constitutes a key milestone towards considerably expanding the computational design envelope currently allowed in industry, where steady-state modelling remains the standard. In this talk, we highlight the key developments that were required to achieve the simulation, from mesh generation to improvements in solver and numerical technology.

[1] G. Mengaldo, et al. "Industry-Relevant Implicit Large-Eddy Simulation of a High-Performance Road Car via Spectral/hp Element Methods." *arXiv preprint arXiv:2009.10178* (2020), SIAM Review November 2021.

15th World Congress on Computational Mechanics (WCCM-XV)
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Entropy Stable Strong Imposition of the No-slip Condition for the Compressible Navier-Stokes Equations

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Key Words: compressible Navier-Stokes, no-slip, entropy stability, injection method

We consider the compressible Navier-Stokes equations which models the motion of a compressible, viscous and heat conducting fluid, in contact with walls. Thus, the equations are augmented with the no-slip condition, leading to the formation of boundary layers, which in turn may become turbulent.

Here, we propose a numerical scheme approximating the compressible Navier-Stokes equations subject to no-slip adiabatic wall boundary conditions. The spatial discretisation is based on the standard second-order finite-difference Summation-by-Parts (SBP) operator. The boundary conditions are imposed using both a weak and strong implementation technique. That is, the Neumann condition for the temperature is imposed weakly using a Simultaneous Approximation Term (SAT), while the no-slip condition for the velocities is imposed strongly via injection. In particular, we focus here on the boundary treatment for the no-slip condition. This weak-strong combination was shown to be stable for the symmetrised, constant-coefficient Navier-Stokes equations in [1]. By using the notion of entropy, we show that it additionally leads to non-linear stability for our proposed scheme.

Numerical simulations are provided to demonstrate the robustness of the boundary treatment for the no-slip condition. A simulation using a fourth-order SBP operator, which yields a linearly stable scheme, is also included.

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Entropy-stable Discretizations for Robust Active Flow Control

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Key Words: Entropy-stable discretization, active-flow control, passivity

We are interested in active-flow control of fluid dynamical systems. Our preliminary goal is to formulate the fluid-control system in such a way that the coupled system remains stable. We leverage passivity theory, which guarantees that the flow-control system is stable with feedback if both the flow and control dynamical systems are independently passive [4]. We briefly show how entropy-stability theory ensures passivity of the continuous fluid system. We then turn our attention to the discretized system and, in particular, stable imposition of boundary conditions at the interface between the actuator and the fluid. To maintain entropy stability, the discretization uses high-order summation-by-parts operators [5] and two-point, entropy-conservative flux functions [6]. Such entropy-stable discretizations are now well established; see, for instance, [3, 2, 1]. The fluid-control framework is demonstrated using an airfoil at a high angle of attack.

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Title: Entropy-stable finite-difference WENO schemes for multiphase flows

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Key Words: Mulitiphase, Entropy Stability, Summation by Parts, WENO, Finite Difference

The multiphase description of flow phenomena represents an attractive option for modeling complex flows because fluid flow over the entire region is modelled using one set of governing equations as opposed to separate sets of equations for each phase [3]. For compressible flow equations in conservative form, in the last decade there have been important advances in the development of provably nonlinearly-stable schemes by combining summation-by-parts (SBP) operators [4] and symmetric two-point flux functions [1]. In this work we look to WENO schemes to automatically provide appropriate upwinding near discontinuities. WENO schemes are capable of attaining arbitrarily high orders of accuracy while sustaining stable and sharp discontinuity transitions [2]. Our goal is to develop provably-stable high-order schemes that render sharp shock interfaces for multiphase flows in non-conservative form. For this purpose, we combine the entropy-stable SBP-WENO framework of Fisher [1] with the entropy-stable framework of Renac [5] to develop entropy-stable SBP-WENO schemes for multiphase flows in non-conservative form. In this presentation, we detail the resulting schemes and present numerical tests on canonical smooth and shocked flows.

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High-Order Implicit Shock Tracking for Time-Dependent Flows

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Key Words: Shock Fitting, Discontinuous Galerkin, PDE-Constrained Optimization

Reference link: https://www.wccm2022.org/submission.html

Shock tracking, as an alternative method to shock capturing, aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter-element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or extensive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features. In previous work [1, 2], we introduced the High-Order Implicit Shock Tracking (HOIST) method that recasts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conservation, stability, and high-order accuracy. By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh.

In this work, the HOIST method is further extended to simulate time-dependent, inviscid flows. We use a space-time formulation of the governing equations and perform shock tracking over a space-time slab for two reasons: 1) it reduces to a steady shock tracking problem over the $(d+1)$-dimensional space-time domain, which allows most of the HOIST framework to be recycled and 2) complex shock-shock interactions simply manifest as triple points. The overall approach is equipped with adaptive time slabs, a procedure to extrude d-dimensional simplex elements over a time slab and split the resulting $(d+1)$-dimensional prism into simplices, and resolution-based h-refinement. The method is demonstrated on a series of increasingly complex unsteady inviscid flows in one and two dimensions.

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Nonlinearly Stable Split Forms for Weight-Adjusted Flux Reconstruction High-Order Methods in Curvilinear Coordinates

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Key Words: Discontinuous Galerkin Methods, Flux Reconstruction, Entropy Stability

The flux reconstruction (FR) method has gained popularity in the research community as it recovers promising high-order methods through modally filtered correction fields, such as the discontinuous Galerkin (DG) method, on unstructured grids over complex geometries. Under a class of energy stable flux reconstruction (ESFR) schemes, FR allows for larger time-steps than DG while ensuring stability for linear advection on affine elements [1]. Alternatively, for nonlinear problems, split forms and two-point entropy conserving fluxes have emerged as the popular approach for unsteady problems on coarse unstructured grids – albeit only having proved stability for the strong form DG scheme and the g_2-lumped Lobatto ESFR scheme for the Euler equations [2, 3]. In this work, we show that incorporating split forms with ESFR schemes, alike Ranocha *et. al.* [2] and Abe *et. al.* [3], generally lead to unstable discretizations. This work is an extension of Cicchino *et al*. [4], where they derived general nonlinearly stable FR schemes in split form for the one-dimensional Burgers' equation and proved stability. This new approach simplifies to ESFR schemes for linear problems, but for nonlinear problems, it ensures nonlinear stability and the correct orders of convergence. This work takes advantage of low-storage weight-adjusted approximations for curvilinear coordinates. The stability of all nonlinearly stable FR schemes are verified with three-dimensional Euler flow in curvilinear coordinates.

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Preparing the path for the efficient simulation of turbulent compressible industrial flows with robust collocated DG-RK solvers

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Key Words: Entropy stable schemes, Robust Runge–Kutta schemes, Cloud Computing

Discontinuous Galerkin (DG) methods are usually infamous for being computationally complex and having robustness issues. However, during the last few years, thanks to the development of entropy stable spatial schemes of any order with the summation-by-parts property, robust and efficient entropy stable nodal versions of the DG schemes have been proposed. However, stability constraints usually limit severely the time step size that can be used to integrate in time the system of ordinary differential equations arising from the spatial discretization with high-order algorithms. These constraints are drastically exacerbated by the i) the mesh element aspect-ratio used to resolve "economically" turbulent flows, and ii) the poor quality of the mesh element for complex geometries.

We present a detailed analysis of the performance of relaxation Runge–Kutta schemes and Runge–Kutta time integration schemes optimized for the spectrum of the semidiscretization of the Euler equations in this paper. The CFL condition or an embedded Runge–Kutta pair are used to combine both time-stepping families with time step adaptivity. When compared to standard and widely used methods for complex industrially relevant turbulent test cases, the new optimized schemes demonstrated an overall speedup of more than 35

Finally, we present a detailed analysis of the performance of the in-house KAUST SSDC framework on the Amazon web service (AWS) cloud computing. The industry is very interested in using this on-demand technology for performing engineering simulations. Thus, testing and assessing the performance of a prototype of next-generation compressible CFD solvers, such as SSDC, is relevant. The results indicate that SSDC scales quite well on the most recent and exotic computing architectures available on the AWS cloud computing platform.

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Space-time hybridizable discontinuous Galerkin methods for incompressible Navier-Stokes

Sander Rhebergen, Tamas Horvath, and Keegan Kirk

In this talk I will discuss a class of space-time hybridizable discontinuous Galerkin method that we introduced and analyzed in [1,2,3,4,5] specifically for the incompressible Navier-Stokes equations. The space-time framework is motivated by our interest in solving the Navier-Stokes equations on time dependent domains, while the hybridizable framework was used to design a space-time discontinuous Galerkin method that is exactly mass conserving (i.e., the discrete velocity field is exactly divergence free on the elements and globally H(div)-conforming) even on moving domains. The exact mass conservation of our discretization has several consequences, such as: local momentum conservation and energy-stability; and the velocity error estimates are independent of the pressure and inverse powers of the viscosity.

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A Data Driven Approach to Improved Exchange-Correlation Functionals in DFT

The need for improved exchange-correlation (XC) functionals in density functional theory (DFT) that can provide quantum accuracy can hardly be overemphasized. To that end, we adopt a data-driven approach to constructing XC functionals by using accurate ground-state densities ($\rho(\mathbf{r})$) from many-body calculations. The key idea is to use the $\rho(\mathbf{r})$ and its corresponding exchange-correlation potential ($v_{\text{xc}}(\mathbf{r})$), from various molecules, as training data to model the XC functional. We present an accurate and robust approach to solve the inverse DFT problem of obtaining the exact $v_{\text{xc}}(\mathbf{r})$ from a given $\rho(\mathbf{r})$, which had, heretofore, remained an open challenge owing to various numerical instabilities in previous attempts. The exact XC potential for seven molecule—dihydrogen at four different bond-lengths, lithium hydride, water, and ortho-benzyne—are computed from full configuration interaction reference densities. These are compared to model XC potentials from non-local (B3LYP, HSE06, SCAN0, and M08-HX) and semilocal/local (SCAN, PBE, and PW92) XC functionals. While for most systems the relative errors in the ground-state densities are $\mathcal{O}(10^{-3} - 10^{-2})$, the model XC potentials have much higher errors of $\mathcal{O}(10^{-1} - 10^{0})$. This finding establishes the utility of the XC potentials—which exhibit greater sensitivity in comparison to the densities—in the design and development of future XC functionals. Subsequently, we use the exact XC potentials to develop neural network (NN) based local and semi-local XC functionals. We provide a comparative study of the NN-based XC functionals against several widely used XC functionals, in terms of their prediction of various thermochemical properties (e.g., atomization energies, reaction barriers, etc).

Development of structure optimization method by quantum annealing

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Key Words: *structure optimization, quantum annealing, quadratic unconstrained binary optimization*

The topology optimization problem is a problem of finding a combination of components that can achieve high performance at low cost. When solving combinatorial optimization problems such as topology optimization problems, local solutions may occur during computation, and the computational cost becomes high if the computation is repeated to obtain the overall optimal solution. Therefore, it is becoming more and more important to develop a computational method to avoid falling into local solutions.

Recently, quantum annealing, a method specialized for solving combinatorial optimization problems, has been attracting attention. Quantum annealing uses the tunneling effect caused by quantum fluctuations to find a solution. Initially, the quantum fluctuation is increased so that the energy exceeds the maximum value due to the tunneling effect, and then the quantum fluctuation is gradually decreased to find the point where the potential is minimized. For example, the previous researches on combinatorial optimization problems using quantum annealing treated applications to traffic volume management and nurse scheduling problems.

Focusing on the minimization of the energy, it is expected that quantum annealing can be used to efficiently obtain globall optimal solutions for topology optimization problems as well. However, no such method currently exists. In this study, we aim to develop a new method for structural topology optimization of solids using quantum annealing. As an example, we take the optimization problem of a truss structure. Specifically, in order to use quantum annealing, the energy of the truss structure is replaced by a Hamiltonian in quadratic unconstrained binary optimization (QUBO) form. The real displacements and cross-sectional areas of the elements need to be expressed in binary variables. Optimization calculations by annealing machine are carried out using the Hamiltonian constructed in this way, and its performance is evaluated.

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DFT-FE --- a massively parallel real-space density functional theory code using adaptive finite-element discretization, and its application to study dislocation core energetics in magnesium

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Key Words: *Electronic structure, Real-space, Spectral finite-elements, Dislocations*

Kohn-Sham density functional theory (DFT) calculations have been instrumental in providing many crucial insights into materials behavior. However, the stringent accuracy requirements in DFT needed to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity with number of electrons, demand huge computational resources. Thus, these calculations are routinely limited to material systems with at most few thousands of electrons. In the first part of this talk, I will present a massively parallel real-space DFT framework (DFT-FE) [1, 2], which is based on a local real-space variational formulation of the Kohn-Sham DFT energy functional discretized with higher-order adaptive spectral finite-element and handles pseudopotential and all-electron calculations in the same framework. We will present the efficient and scalable numerical algorithms in conjunction with mixed precision strategies for the solution of Kohn-Sham equations, that has enabled computationally efficient, fast, and accurate DFT calculations on generic material systems reaching ~100,000 electrons and demonstrate an order of magnitude performance advantage over widely used plane-wave codes both in CPU-times and wall-times. In the second part of this talk, I will present the application of DFT-FE to study the core energy difference between the <c+a> screw dislocations on pyramidal I and II planes in pure magnesium (EpyrI-II). EpyrI-II forms a crucial and sensitive input to a quantitative model predicting the ductility of magnesium alloys. However, accurate estimation of EpyrI-II using explicit DFT calculations has so far been out of reach using plane-wave codes as large system sizes containing thousands of atoms are required to accurately resolve the relevant physics in the dislocation core. Using DFT-FE, we conduct a systematic cell size study of EPyrI-II till ~3,500 atoms (35,000 electrons) per periodic layer along the dislocation line. We find that a cell-size of ~2,700 atoms is required to obtain EPyrI-II under a cell-size error of 5 meV/nm. We also find strong influence of external macroscopic uniaxial deformations on EPyrI-II. Obtaining EPyrI-II accurately has significant implications for designing highly ductile magnesium alloys.

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FEqa: Solving Finite Element Problems using Quantum Annealing

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Key Words: *Quantum Computing, Quantum Annealing, Finite Element Method, Iterative, Cosine Measures*

Quantum computing is a rapidly developing area of research with potential applications extending over scientific and engineering computation. Current work in quantum computing for partial differential equations is sparse and limited in scope with presently available Noisy Intermediate Scale Quantum (NISQ) hardware. Quantum annealers are NISQ devices designed to minimize the Ising Hamiltonian. Current demonstrated applications of quantum annealers suffer from various forms of inefficiencies. Here, we explore the application of quantum annealing to finite element problems and develop a unified general framework to iteratively solve linear partial differential equations with examples problems solved on D-Wave quantum annealer.

A general methodology to map finite element problems to the Ising Hamiltonian is developed by a novel generalization of the Ising Hamiltonian and posing the finite element problem as a minimization problem. Several novel mapping options are developed, and their strengths and weaknesses explored. Procedures that efficiently map one unknown to one qubit with sparse graphs are presented. A time-efficient scheme is presented to calculate the mapping by parallelizing over the elements.

Novel iterative procedures are developed to iteratively carry out the finite element minimization problem using quantum annealers, dubbed as the single step "2^N Search", "3^N Search", and the two-step "Hyperoctant Search". A general framework to develop higher order iterative procedures is presented in the context of Nested Iterations. Since these iterative procedures differ significantly from classical procedures by sampling from exponentially large sets, their mathematical properties are explored with proofs of their cosine measures to outline their effectiveness compared to classical methods. An exponential increase in cosine measures is demonstrated, highlighting the potential for quantum annealing to iteratively solve minimization problems with classically intractable numbers of unknowns.

The iterative procedures are carried out for example problems using classical simulated annealing and quantum annealing for a head-to-head comparison of classical and quantum techniques. The annealing time for simulated annealing grows as O(N), whereas it is O(1) for quantum annealing [1] (King et al., 2015), though they have similar convergence rates. The Hyperoctant Search procedure demonstrated the best convergence properties with some instances of super-convergence with only 10^1 anneals per iteration compared to 10^3-10^6 anneals typically needed for other methods.

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Finite-element based methodologies using projector augmented wave approach (PAW) for large-scale density functional theory calculations

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Key Words: Finite-elements, DFT, PAW method, extreme-scale computing

Quantum modeling of materials, in particular density functional theory (DFT) calculations have provided many crucial insights into materials behavior over the past few decades and occupy considerable fraction of world's computational resources today. However, asymptotic cubic-scaling computational complexity with number of atoms in conjunction with stringent precision requirements for accurate material property prediction demand huge computational resources for these calculations. Thus, these calculations are routinely limited to material systems with few hundreds of atoms, employing plane-wave discretizations despite its limitations. The development of DFT-FE [1,2], a massively parallel open-source DFT code addresses these challenges by making use of higher-order spectral finite-elements alongside with novel HPC centric numerical strategies focusing on significantly reducing the data movement costs and increasing arithmetic intensity on evolving hybrid CPU-GPU architectures. These methodologies enabled systematically convergent, fast and scalable norm-conserving pseudopotential DFT calculations using real-space finite-element (FE) based methods on material systems involving tens of thousands of electrons for both metallic and insulating systems, on massively parallel computing architectures, while allowing for arbitrary boundary conditions and complex geometries. However these recent advances are limited to norm-conserving pseudopotentials (ONCV, TM) and are not applicable to DFT calculations using projector augmented wave (PAW) method in a straight forward way. The widely used PAW frozen-core method for DFT is shown to be highly transferable and deals with much smoother electronic fields thereby resulting in huge reduction in degrees of freedom in comparison to their norm-conserving pseudopotential counterparts. To this end, we will present a real-space DFT formalism within the PAW framework amenable to higher-order spectral finite-element discretization. Furthermore, accuracy and performance of the proposed approach on hybrid CPU-GPU architectures will be demonstrated on a variety of benchmark examples including large-scale materials systems involving few thousands of electrons

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Modeling of Complex Nanostructures using a Large-Scale DFT code CONQUEST

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Key Words: *O(N), linear-scaling DFT, local orbitals, nanoscale materials, machine learning*

Although density functional theory (DFT) is a powerful tool to clarify the atomic and electronic structures of materials, DFT studies of complex nanostructures are usually very difficult because conventional DFT methods cannot treat large systems containing many thousands of atoms. To overcome this problem, we have developed a large-scale, linear-scaling DFT code CONQUEST, which has recently been released under an open-source MIT license. The code uses local orbital and linear-scaling methods, and has high efficiency on massively parallel computers.

In this presentation, we explain the theory behind the code and survey the recent developments and applications of CONQUEST. It will be demonstrated that CONQUEST can calculate the atomic positions of the realistic models of nano-scale materials observed in experiments and can clarify the unique electronic properties of these complex materials. A new method based on the machine learning techniques to analyze the local atomic structures observed in large-scale DFT-MD simulations will be also discussed.

This work has been done in collaboration with D. R. Bowler, J. S. Baker, S. Y. Mujahed, J. T. L. Poulton (UCL, UK), A. Nakata, M. Tamura, J. Lin, Z. Raza, S. Yadav, S. Arapan (NIMS, Japan), L. Truflandier (U. Bordeaux, France), M. Matsuda, Y. Futamura and T. Sakurai (U. Tsukuba, Japan).

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Practical Boundary Conditions for Electronic Structure Calculations

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Key Words: *Boundary Conditions, Symmetry, Density-Functional Theory*

Computational materials design is an active area of research which aims at predicting physical and chemical properties of various materials from first-principles electronic structure calculations. To keep the computational costs manageable, the Schrödinger equations are often approximated by Kohn-Sham equations within the framework of density-functional theory [1]. These Kohn-Sham equations are solved numerically either by a basis set expansion or real-space discretization under given boundary conditions. In the case of a plane-wave basis set, it is common practice to apply periodic boundary conditions in all directions [1], while isolated boundary conditions are more common for the atomic basis set. However, there are many other options besides these standard boundary conditions. In this talk, we will explore several non-standard boundary conditions which exploit the characteristics of each system, such as surfaces, interfaces, and cyclic/helical structures, to minimize the computational costs of electronic structure calculations. Most of these boundary conditions are easily implemented by minor modifications of existing electronic structure codes. Numerical examples on a few model systems are also presented for the validation of these boundary conditions.

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Simulation of the phase-separation structure of a diblock polymer using Ising machine

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Key Words: *Quantum Annealing, Ising Machine, Microtructure, Diblock Polymer, Computer Simulation Acceleration*

A diblock polymer is a polymer in which two different homopolymers are connected to form a single polymer. In diblock polymers, the phase separation of the two different homopolymers forms microstructures. The microstructures change depending on the experimental conditions, such as lamellar, cubic, hexagonal, and gyroid structures. Since the microstructures have a significant effect on the mechanical properties of the polymer, it is important to predict which type of microstructure will appear under the given experimental conditions. To date, several methods have been developed to predict the microstructures[1], however, conventional methods sometimes take a long time to obtain the prediction.

In recent years, Ising machine have attracted much attention to solve the combinatorial optimization problems. Ising machine solves quadratic unconstrained binary optimization (QUBO), which is one of the formalized combinatorial problems; in QUBO, the variables is a set of binary states, and the objective function, called Hamiltonian in the context of the Ising machine, consists of up to a quadratic polynomial of the binary states. Since the Ising machine solves the states where the value of the Hamiltonian is minimized, the problem to be solved should be mapped to a QUBO-style problem, in other words, the coefficients of the quadratic polynomial of the Hamiltonian are configured.

In this work, we proposed a new method to perform two-dimensional simulations of the phase-separation structure of a diblock polymer using the Ising machine. We mapped the problem of performing the simulation to the Hamiltonian as a sum of four quadratic terms that represent different physical behavior of diblock polymers: the sum amount conservation term, the Flory-Huggins interaction energy term, the gradient energy term, and the Ohta-Kawasaki long-distance interaction energy term. By adjusting each term, different experimental conditions can be represented.

Using the proposed method, we observed several types of phase separation such as dotted and striped patterns, which correlate to lamellar and cubic or hexagonal structures. Together with other results, the proposed method was shown to be successful to predict the microstructures. Furthermore, each simulation using the Ising machine takes less than 1s, which is hundreds of times faster than conventional methods.

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A mesh-less, ray-based Deep neural network method for the Helmholtz equation with high frequency

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Key Words: *Deep Learning; Plane wave; Deep Neural Network; Loss; High frequency; Helmholtz equation.*

We develop a mesh-less, ray-based deep neural network method to solve the Helmholtz equation with high frequency. This method does not use an adaptive mesh refinement method, nor does it design a numerical scheme using some specially designed basis function to calculate the numerical solution, but it has the advantages of easy implementation and no mesh. We have carried out various numerical examples to prove the accuracy and efficiency of the proposed numerical method.

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A spectral approach for time-dependent PDEs using machine-learned basis functions

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Key Words: Spectral methods, deep operator networks

A major obstacle in the deployment of spectral methods is the choice of appropriate bases for trial and test spaces. If chosen suitably, these basis functions lead invariably to well-posed discretized problems and well-conditioned linear systems, while the resulting approximate solutions are provably high-order accurate [1]. However, barring domain decomposition approaches, devising such functions for arbitrary geometries from scratch is a hugely challenging task [2]. Fortunately, the recently developed DeepONet approach is a highly promising device for generating machine-learned basis functions [3]. In this talk, we propose a Galerkin approach for time-dependent PDEs that is powered by basis functions gleaned from the DeepONet architecture. We shall outline our procedure for obtaining these basis functions and detail their many favourable properties. Next, we shall present the results of numerical tests for various problems, including advection, advection-diffusion, viscous Burgers' equations, as well as some highly intriguing preliminary results from the low-viscosity regime. Finally, we will identify potential pitfalls in the course of generalization to higher dimensions and suggest possible remedies.

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Adaptive integration to overcome quadrature problems in Neural Networks

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Key Words: Deep learning, Neural Networks, Ritz method, Least-Squares method, Quadrature rules.

Neural Networks have been widely used to solve Partial Differential Equations (PDEs). In there, definite integrals are required to be solved. Deep Neural Network (DNN) techniques present several advantages and limitations with respect to traditional PDE solvers based on Finite Elements, Finite Differences, or Isogeometric Analysis. Among the advantages of DNNs, we encounter the nonnecessity of generating a grid. In general, DNNs use a dataset in which each datum is independent from others. In contrast, in the linear system that produces the FEM method there exists a connectivity between the nodes of the mesh. Furthermore, DNNs provide the possibility of solving certain problems that cannot be solved via traditional methods, like high-dimensional PDEs, fractional PDEs, and multiple nonlinear PDEs. However, DNNs also present limitations when solving PDEs. For example, the convergence of the method is often assumed (see, e.g., [1]) since it cannot be rigorously guaranteed due to the non-convexity of the loss function. Another limitation is the lack of proper quadrature rules for integrating functions coming from DNNs [2].

This works analyzes the problems associated with quadrature rules in DNN methods when solving PDEs. In particular, we illustrate with a simple one-dimensional Poisson problem the disastrous consequences that may appear as a result of an inadequate selection of a quadrature rule. We propose an alternative to overcome the quadrature problems: adaptive integration. We are able to control the quadrature errors by adding new quadrature points to the training dataset. Implementation of this strategy requires the use of meshes, which posses a limitation on high-dimensional integrals. As an alternative to generating a mesh, one can add points using clustering algorithms to the training set, but this entails difficulties when designing an adaptive algorithm.

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Bayesian Optimization for Simulation Errors Under Time Constraints

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Key Words: Bayesian Optimization, Constrained Optimization, Multi-Scale Simulation

The muscle simulation framework OpenDiHu [3] consists of many numerical components on multiple scales [1]. Their combination and interaction directly influences the simulation accuracy and computational time. However, finding an optimal combination of these components that balances accuracy and computational resources can be a difficult and time consuming process.

Model-based Bayesian optimization is a useful tool to tackle such problems [2]. We present a Bayesian approach to optimize the temporal discretizations on multiple scales of the simulation for a minimal error under run time constraints. In each step of the Bayesian optimization, a model for the simulation error and the run time is improved. This model uses already known samples of the simulation behavior and incorporates prior knowledge of the simulation such as a-priori convergence orders and run time scaling of the components. To update the model with a new data sample, the simulation is executed with new discretization parameters. These are selected by an acquisition function based on the model prediction and uncertainty. A new data sample should not only help to approach the optimum of the objective function, but also improve the models that are used for the optimization. As the simulation error and the run time are unknown for unevaluated samples, the acquisition function also has to select samples that improve the model quality, i.e., the models for both the discretization error and the run time. We discuss our optimization approach, modeling aspects and choices for the acquisition function.

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r-adaptivity Deep Learning method for solving Partial Differential Equations

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Key Words: Neural Networks, r-adaptivity, Deep Ritz Method, Partial Differential Equations

In the last five years, the research on the use of Deep Neural Networks (DNNs) to solve partial differential equations (PDEs) has intensified [1]. Some traditional methods used in this context are: the Deep Ritz method [2], the Deep Least-Squares method [3], and the Deep Galerkin method [4]. These methods are often mesh free due to the use of a Monte Carlo type integration. However, in low dimensions (three or below), Monte Carlo integration may lead to slow convergence rates and other integration methods may be preferred. In particular, mesh-adaptive methods may deliver faster convergence while ensuring proper integration in context of DNNs.

Herein, we propose an r-adaptive DNN method. For illustration, we consider a Deep Ritz method with a piecewise-polynomial solution over a tensor product mesh. During the training of the DNN, we simultaneously optimize the node positions (r-adaptivity) and the solution. This method does not require a posteriori error estimation. It also allows to fix some mesh points, which may be convenient for establishing material boundaries. Our method allows for topological changes and does not need to maintain the connectivity between elements as in the Finite Element Method. Numerical results show the behaviour of the method in one- and two-dimensional domains for solutions that are smooth, singular, or have a strong gradient.

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Smooth approximation of physics using Deep Neural Networks and Isogeometric Analysis

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Key Words: *Deep Neural Networks, Isogeometric Analysis, Physics Informed Neural Networks*

We compare the application of Deep Neural Network (DNN) for approximation of the solution of Partial Differential Equations (PDE) using three different methods. The first method is based on our proposition of using the linear combination of higher-order and continuity B-spline base functions and employing the DNN to approximate B-splines' coefficients. The second method is based on using the DNN for direct approximation of the solution of PDE obtained from isogeometric analysis (IGA) (finite element method employing B-spline base functions).
Solving differential equations with neural networks has been proposed by Maziar Raissi et al. in 2017 [1] by introducing Physics-informed Neural Networks (PINN), which naturally encode underlying physical laws as prior information. Thus, we also compare the first method to the PINN approximation. Approximation of coefficients using a function as an input leverages the well-known capability of neural networks being universal function approximators, as shown by Hornik et al. in [2]. In essence, in the PINN approach, the network approximates the value of the given field at a given point. Alternatively, the DNN can approximate the IGA solution pointwise. We present an alternative approach, where the physical quantity is approximated as a linear combination of smooth B-spline basis functions, and the neural network approximates the coefficients of B-splines. This research compares results from the DNN approximating the coefficients of the linear combination of B-spline basis functions, with the DNNs approximating the solution directly. We show that our approach is cheaper and more accurate when approximating smooth physical fields [3].

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A Dynamically Aggregated Decomposition Strategy for High-dimensional Global Optimization

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Key Words: *Efficient global optimization，Large-scale optimization，Surrogate model*

Abstract The efficient global optimization (EGO) algorithms, which are well-known to be sample-efficient, have been extensively used for solving expensive black-box problems in various scenarios. However, due to the "curse of dimensionality", most EGO algorithms can only work well for optimization over domains of less than 15 dimensions [1], it is quite challenging to scale EGO algorithms for solving problems of even higher dimensions (e.g., d > 30). Divide and conquer is a common idea to address the above issue [2], which decomposes the original problem into several low-dimension subspaces and handles each sub-problem independently with EGO. Considering the interactions of variables, the decomposition strategy is of vital importance. However, the subspaces are determined before the optimization process in most of the previous studies, which can be quite expensive to achieve it.

To address this problem of decomposition in a more efficient way, a new optimization algorithm with novel decomposition strategy is proposed, called dynamically aggregated EGO algorithm (abbreviated as DA-EGO). The characteristic of this method is that accurate decomposition is achieved step by step in the optimization process rather than in one shot. At the beginning, the high-dimensional problem is completely divided into one-dimensional sub-problems. And then, the strongly correlated variables are aggregated into groups, while the weakly correlated variables are pruned directly. More specifically, the global and local surrogates bear the functions of nomination and confirmation respectively. The global model is established with Polynomial chaos expansion（PCE) using all evaluated samples, whose coefficient directly represents the interactions between variables. When a pair of variables is nominated, they will jointly establish a local Kriging model and confirm their relevance in the next round of optimization. More and more correlations are determined as the optimization progresses. Under this operation, the optimization gradually changed from a general independent optimization of all variables to a focused optimization of several clusters of aggregated groups.

We test our proposed DA-EGO algorithm on 12 benchmark functions. The results of DA-EGO are shown significantly better than other compared the state-of-the-art algorithms. And hence, the effectiveness of our proposed algorithm is well demonstrated.

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Buckling Analysis of Stiffened Thin-Walled Structures Using a Novel Beam-Shell Isogeometric Model

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Key Words: *Isogeometric analysis, Stiffener element, Degenerated element, Stiffened thin-walled structure, Buckling analysis*

Stiffened thin-walled structure is one of the most improtant structural forms in lightweight design. Highly accurate and efficient analysis methods are the basis of structural design. For the standard faceted finite element theory, typical finite element meshes introduces geometric imperfections. Only refinement of the mesh can reduce geometric errors. Therefore, accuracy and efficiency are contradictory in classical finite element analysis (FEA). This will require a change from classical FEA to an analysis procedure based on CAD representations. Hughes et al.[1] first introduced the isogeometric analysis (IGA) based on NURBS basis function. Considered as a feasible alternative to polynomial based finite element analysis, IGA effectively solves the problems of high cost, time-consuming and geometry error in the construction of standard finite element analysis mesh. Therefore, in this paper, a general, simple and efficient isogeometric analysis method for stiffener thin-walled structures is proposed. Both shell element[2] and stiffener element are based on degenerated 3D elements theory. The skin of stiffened thin-walled sturcture is a shell with arbitrary geometry. Therefore, NURBS surface is used to build an accurate geometric model of the skin. Stiffeners are modeled with NURBS curves. Degeneration theory started from continuous mechanics, avoiding complex theoretical assumptions and derivation of formulas. At the same time, high-order NURBS basis functions can avoid shear self-lockling of the shell element and stiffener element, so such theories are applicable to arbitrary thickness and section size. In this paper, the method proposed by Kapnia et al.[3] is used to couple the degrees of freedom of the skin and stiffener. NURBS surface can provide the normal vector at any point. These geometric algorithms greatly reduce geometric errors. Numerical results indicate the present method has good accuracy, efficiency and robustness.

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Elastic Buckling of Cylindrical Shell Subjected Pressure Load at Surface

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Key Words: Buckling, Eigenvalue Analysis, Internal/External Pressure, Shell Element

Cylindrical shell is employed in a wide range of fields including pressure vessels, storage tanks, submarines, and aircraft fuselages. In these shell structures, buckling may occur due to various loading, such as compression, bending, twisting, shearing, and internal and external pressures. When the internal and external pressures are applied to both the top and bottom surfaces of these shell structures, the behavior is different from the case where the pressure acts on either the top or bottom surface[1].

Buckling phenomena of structures under pressure load are studied with the finite element analysis. Toscano et al.[2] proposed the finite element model discretized with shell elements for analyzing the buckling and buckling propagation of stiffened pipes, and verified the developed model by comparing the numerical results obtained using it with the experimental data. In this approach, the pressure load is evaluated at the midsurface of shell structure. On the other hand, in order to evaluate the pressure load appropriately, Zhu et al.[3] presented the numerical calculation considering the three dimensional finite deformation for the thick-walled cylindrical shell in the buckling analysis. However, it needs huge computational costs to represent the complicated behaviors using continuum elements.

In this work, we propose a numerical procedure using the special shell element[4], in which the external force is directly given to the additional nodes representing the thickness–stretch, to evaluate the buckling behavior of the cylindrical structure subjected to pressure load, in the framework of structural elements. Since the discontinuities of the thickness between elements are allowed, the number of unknowns in the resulting linear system of equations is coincide with that of conventional shell elements by employing static condensation in constructing the element stiffness matrix. In the case of applying a perturbative load under a certain stress state, bifurcation points are searched by solving a standard eigenvalue problem.

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Global buckling design optimization of spatially graded grid-stiffened plates based on asymptotic homogenization

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Key Words: *Grid-stiffened plates, spatial gradation, buckling optimization, asymptotic homogenization*

Grid-stiffened plates are widely employed in engineering applications due to light weight, high specific stiffness/strength and are quite competitive in terms of structural stability. Conventional grid-stiffened plates are designed to be uniformly distributed microstructures, and structural performance is significantly confined as spatial gradation of stiffener layout is prohibited in the design space.

In this work, a two-step multiscale optimization for spatially varying stiffener layout is conducted to enhance structural buckling resistance based on asymptotic homogenization. In the first step, the stiffener orientation and material layout are first optimized in the macro scale. In the second step, mapping functions are introduced to map the original uniform microstructure into a spatially varying stiffened plate, and geometric features of stiffener layout, such as stiffener spacing, stiffener length parameters, are established with mapping function parameters. Then a mixed optimization formulation, which integrates mapping functions into the eigenvalue buckling load factor, is proposed for maximum stability performance, and concurrent optimization for mapping functions and stiffener layout is conducted. The advantage of this formulation is two-fold. First, the design space is relaxed so that structural performance can be improved to a large extend. Second, a good agreement, in both shape and performance, between the projected single-scale stiffened plate and the homogenization results is expected. At last, de-homogenization procedure is carried out to visualize the graded stiffened plate and eigenvalue buckling analysis is performed to show the validity of the optimization results.

Several numerical examples are presented to show the validity of the proposed method and the results are compared with regularly distributed stiffened plates to demonstrate the potential of spatially graded stiffener configurations in improving structural stability performance.

Isogeometric Stability Analysis of Thin-Walled Structures

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Key Words: *Shell Buckling, Isogeometric Analysis, imperfections, dynamic buckling*

The load carrying capacity of thin-walled structures is known to be significantly influenced by stability aspects such as buckling. A reliable prediction of buckling phenomena requires a robust and accurate analysis tool and consideration of a number of inherent structural imperfections which often dominate the overall non-linear elastic response.

In this contribution, we present buckling and post-buckling problems of thin-walled structures in the framework of isogeometric analysis of isotropic and laminate composite shells considering geometric imperfections. Our approach exploits the higher order approximation and continuity properties of NURBS modelled shell structures and considers arbitrary openings and cut-outs, as common in industrial applications, on the basis of the finite cell method. The latter proved to be an efficient fictitious domain extension to isogeometric analysis in the context of trimmed NURBS geometries. In particular, the fictitious domain extension allows for a simple and flexible consideration of multiple cut-outs of arbitrary shape from the shell body and at arbitrary location without any re-meshing. Thus, it provides a powerful tool for the systematic study of the buckling tendency of industry relevant models. We will present a number of challenging shell buckling problems to reveal and assess the reliability and accuracy of a fictitious domain extended isogeometric analysis approach of geometric imperfect thin-walled structures.

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Model-Data-Driven Hybrid Computational Framework for Large Deformation Analysis

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Key Words: *data-driven, model-driven, large deformation*

The Data-Driven Computational Mechanics, proposed by Kirchdoerfer and Ortiz[1], is a novel computing paradigm in which the constitutive model is replaced by the material data set. Compared to the conventional "model-driven" computing, it can eliminate the error and uncertainty in material modeling, but may have expensive computational cost and poor convergence in certain situations[2], such as instability under large deformation. Hence, We propose a novel hybrid computational framework for large deformation analysis, combining the "model-driven" and "data-driven" algorithms. In the "model-driven" part, an empirical constitutive model is firstly calibrated with material data set and the preliminary solutions are obtained based on the finite element method. The above solutions are used as the initial iterations in the "data-driven" part, where the distance-minimizing data-driven algorithm is implanted to find the best solutions in the material data set that are closest to satisfying the equilibrium. The equilibriums with large deformation are nonlinear and solved by the Newton-Raphson method. The advantages of both the two algorithms can be gathered, where the robustness is ensured and the uncertainty of material model is eliminated. Since the initial iterations under each loading stage have already been obtained in "model-driven" part and are independent of each other, parallel computing can be used to significantly improve the efficiency of the "data-driven" computing part. This work can provide an efficient and robust tool for analysis and design of advanced materials.

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NEW CREATION OF ORIGAMI BASED ON BIFURCATION ANALYSIS FROM FULLERENE STRUCTURES

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Key Words: Post-buckling, Origami skill, Bifurcation, Fullerene, Imperfection

The form of the *Buckminster fullerene* as geodesic sphere and other fullerene molecular such as Carbon 60(C_{60}), nano-tubes in nano-micro-macro scale structures has become popular among architects and/or chemists[1, 2]. The icosahedral symmetry of its structure, which is rarely found in nature, is difficult to analyse in scale-range physics problem. The analysis of these highly symmetric structures gives rise to a nonlinear problem with a singularity such as bifurcation problem[3], post-buckling problem in engineering and science. The authors therefore put forward a method to analyse the perfect structures, however, its imperfect one is more complicate to analyse bifurcation problem of fullerenes. Compared with the perfect system, the small deviation of the initial value will have a great impact on the subsequent situation, making the buckling process evolve in a completely different way.

In this study, the fullerene structure is studied from local to global. The elastic post-buckling analysis of frame, hemisphere and whole model is carried out respectively. In other words, even if there is only one part of the structure, the state of local buckling is taken as the service limit and the state of buckling in other places is taken as the final limit, so that the dangerous state can be understood in stages. From the perspective of structural symmetry classification, the initial shape of the structure can be changed by adding the imperfection of different nodes to produce the expected local defects. By reducing the symmetry of the structure gradually, the stiffness curve corresponding to the buckling process of the structure is measured by using arc length method. It is found that based on the original primary path, there are different bifurcation paths.

In summary, the post-buckling process of the fullerenes adds imperfection through Origami mechanism[4] to track the geometric deformation in the bifurcation phenomenon. Analytical results are used to further improve the laws of bifurcation mechanism with imperfection problem in symmetric structures. It is possible to create a folding system and stronger design based on this approach[5].

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Stochastic Isogeometric Buckling Analysis of Complex Thin-walled Structures with Random Material Properties

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Key Words: *Isogeometric analysis, Uncertain Analysis, Karhunen-Loève Expansion, Perturbation Method*

With the rapid development of advanced manufacturing technology, various complex thin-walled structures are fabricated and utilized in engineering fields such as aerospace. However, the traditional finite element method (FEM) produces geometric errors due to meshing. And at the same time, the randomness of system parameters is inevitable in the manufacturing process [1]. Herein, a new stochastic method, referred to as stochastic isogeometric analysis (SIGA) considering the uncertainty of the material properties, is proposed to solve the stochastic linear stability problem of complex thin-walled structures. Isogeometric analysis [2] is highly promising and efficient numerical analysis method, and is adopted as a deterministic solver for governing partial differential equations. The Gaussian random fields with spatial variability of material properties are represented by Karhunen-Loève expansion, which is a linear combination of a set of independent random variables and orthogonal functions. The orthogonal functions and corresponding eigenvalues are obtained by solving the Fredholm integral equation of the second kind by the Galerkin isogeometric method [3]. This method exploits the regularity of NURBS basis functions delivering globally smooth eigensolutions and the total mean squared error of the random field is minimized simultaneously. Since the autocovariance function of the response solution is unknown, the perturbation method is developed to solve the stochastic linear buckling equation and predict the second-moment statistics of the buckling load. To verify the validity and applicability of the proposed method, two numerical examples including metallic and composite shells are presented. The accuracy and efficiency of the results are assessed by independent Monte Carlo simulation based on the IGA algorithm, and proved that the proposed method can effectively obtain the mean and standard deviation of the buckling load, thereby efficiently determining the strength limit of the shell structures.

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STRUCTURAL INSTABILITY OF MULTIPLE MICRO-PERIODIC STRUCTURES

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Key Words: Hill-top bifurcation, Multiple bifurcation, Bifurcation theory

Fundamental mechanism for the global and local (un-)stabilities based on geometrically periodic micro-macro structures and/or materials such as porous bodies, honeycomb, between the scales of atomic lattice structure and crustal deformation of geological folding under compression loading are reviewed from a post-buckling perspective. This folding phenomenon in nonlinear mechanics appears beyond the physics of scales problem as multi-body dynamics [1, 2]. In the viewpoint of multi-body physics issues, the structure is assumed that the mechanical model of the multi-folding micro-structure (MFM) [3] in a closed boundary condition is allowed to fold to a stable state through sequential unstable states such as snap-through or snap-back phenomena and deflections are considered so far into the large-deformation range. It is well-known the classification of single bifurcation point such as limit point, symmetry/asymmetry or stable/unstable bifurcation and so on. There is a hilltop branching point occurring as a coincidence of a limit point and arbitrary many bifurcation points of a finite-dimensional, elastic, conservative and equivariant system to its symmetry. The mechanical and elastic model of the MFM are derived for finite dimensional elastic conservative systems exhibiting hilltop branching at which arbitrary many bifurcation points coincide with a limit point. We have investigated the classification and/or bifurcation paths of multiple bifurcation point at hilltop (un)stable bifurcation point for structural model with periodic structure. The imperfection sensitivity with the hill-top bifurcation point displays complex phenomena of the geometrical nonlinearlity of multi-folding elastic model. We have investigated structural instability of the multiple (a)symmetry bifurcation paths from hilltop limit point in MFM model with periodic symmetry and/or loss-symmetry in the case of bridge collapse and/or periodic micro-macro structures.

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The Koiter-Newton method for thermal-mechanical buckling and postbuckling analysis of thin-walled structures

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Key Words: Koiter-Newton method, Temperature field, Thermal-mechanical buckling, Reduced-order model

Thin-walled structures suffer a complex buckling failure under the thermal-mechanical environment. The initial stresses induced by the thermal expansion may lead to an "early buckling" for the structure.

The reduced-order modeling method, termed as the Koiter-Newton method, is reformulated to be applicable for geometrically nonlinear thermal-mechanical analysis of thin-walled structures. The initial temperature field over the whole structure is converted into the thermal load imposed on the structural nodes. The thermal load is treated as the independently unchanged load corresponding to the initial temperature field. The internal force space is expanded using the mechanical load, the thermal load and the predefined perturbation loads. The thermal-mechanical reduced-order model is constructed using the first to fourth-order derivatives of strain energy with thermal effects in terms of the degrees of freedom. An additional degree of freedom related to the thermal load appears in the construction of reduced-order model based on the novel Koiter theory. The path-following scheme is proposed to make the method able to trace the entire geometrically nonlinear thermoelastic response. A much larger step size can be achieved benefiting from the favorable prediction of the reduced-order model, compared to the classical Newton-like methods.

Numerical results validate the excellent performance of the proposed method in thermal-mechanical buckling analysis. The flat plate and curved panel with isotropic or orthotropic materials are selected considering the initial temperature fields. Firstly, the accuracy of the proposed method on tracing the geometrically nonlinear thermoelastic response is well guaranteed compared to the classical Newton-like methods. Much less number of steps is required for the proposed method attributing to the favorable predictor provided by the reduced-order model. A single step is enough for the flat plate with almost linear prebuckling behavior, to achieve the response satisfactorily up to the buckling load as well as the initial postbuckling region, while a few more steps may be needed for the curved panel that shows significant prebuckling deformation. Then, the thermal-mechanical buckling and postbuckling analyses of thin-walled structures are carried out using the proposed method. The influences of boundary conditions, uniform/nonuniform temperature fields and temperature-independent/dependent material properties on thermal-mechanical buckling behaviors are carefully studied. We conclude that the proposed method is a general, highly efficient and robust numerical method for geometrically nonlinear thermal-mechanical buckling analysis.

Uncertainty quantification method for geometric imperfections of cylindrical shells based on multi-Chebyshev envelope model

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Key Words: *geometric imperfections, uncertainty quantification，limited samples, cylindrical shell*

Thin-walled cylindrical shells are widely used as main load bearing structures in the aerospace industry. Considering the high sensitivity of the buckling load to initial imperfections, especially geometric imperfections, the prediction of the knockdown factor is crucial to both structural safety and lightweight design. However, the generation of geometric imperfections is influenced by many factors, particularly the manufacturing process, whose complex distribution and spatially varying uncertainties are quite difficult to be described. The inherent strong random characteristics of geometric imperfections seriously expose the drawbacks of conventional deterministic knockdown factor prediction methods. Therefore, to obtain the load-bearing characteristics of the cylind1er shell under stochastic imperfections, there is an urgent need to conduct in-depth research on uncertainty quantification methods of geometric imperfections first. To overcome abovementioned challenges, a novel multi-Chebyshev envelopes (MCE) model is proposed in this paper. It can cover the stochastic properties of geometric imperfections with limited samples. The numerical results demonstrate that the MCE model achieves excellent performance in the accuracy of uncertainty quantification of geometric imperfections. Finally, a high-fidelity uncertainty quantification model of measured geometric imperfections of cylindrical shells is obtained by proposed method in a rational and objective manner.

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A Two-Step Quadratic Spline Collocation Method for the Biharmonic Dirichlet Problem in Two Dimensions

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Key Words: Biharmonic Dirichlet Problem, Quadratic Spline Collocation, Fast Fourier Transforms, Optimal Global Convergence Rates, Superconvergence.

Optimal quadratic spline collocation (QSC) methods were first developed in [4] for solving second-order two-point boundary value problems. Two methods were considered, a one-step or extrapolated method, and a two-step or deferred correction method. Both methods were extended to second-order elliptic boundary value problems in two space variables in [3], and to parabolic problems in one space variable in [2]. In this presentation, a two–step QSC method is described for the solution of the Dirichlet biharmonic problem on the unit square rewritten as a system of two second-order partial differential equations. This is commonly known as the mixed approach. The method involves fast Fourier transforms and, in comparison to its one-step counterpart given in [1], it has the advantage of requiring the solution a symmetric positive definite Schur complement system rather than a nonsymmetric one. The total cost of the method on a $N \times N$ partition of the unit square is $O(N^2 \log N)$. Although third-order accurate globally, the QSC solution is fourth-order accurate at the nodes of the mesh on which it is defined. This is the same nodal accuracy as that of optimal methods based on cubic spline collocation, which involve four times as many unknowns. Numerical results demonstrate this accuracy of the QSC method.

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Convergence of finite difference schemes for biharmonic time-dependent problems

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Key Words: Finite differences, compact schemes, Stephenson scheme, biharmonic, Navier-Stokes equations, streamfunction

We consider various time dependent parabolic biharmonic problems in a square which appear in fluid dynamics, including models for the Navier-Stokes equations in streamfunction form. We approximate these time-dependent problems in space by finite difference compact high-order schemes. The finite difference scheme handle these problems without decoupling the biharmonic operator into two Laplacian operators. The compact high-order schemes which we apply to the biharmonic problems display interesting properties of stability and accuracy. Typically, our schemes exhibit fourth-order convergence rates, even when the truncation is less than fourth-order at certain nodes. We prove that for the semi-discrete problem, which is discrete in space and continuous in time, the scheme is fourth-order accurate. The proof invokes various matrix analysis techniques, which may be useful in other contexts. In the talk, we will review the diversity of these matrix techniques.

The talk is related to the references [1, 2].

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Finite-element discretization of the smectic density equation

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Key Words: Biharmonic equation, H^2-conforming element, C^0 interior penalty method, mixed finite-element method

Fourth-order PDEs arise in many settings, including in models of thin plates and shells and of some liquid crystalline materials. The density variation of smectic A liquid crystals[4] is governed by such a fourth-order PDE, which exhibits two complications over the biharmonic or other typical H^2-elliptic fourth-order problems. First, the equation involves a "Hessian-squared" (div-div-grad-grad) operator, rather than a biharmonic (div-grad-div-grad) operator. Secondly, while positive-definite, the equation has a "wrong-sign" shift, making it somewhat more akin to a Helmholtz operator than an elliptic one. In this talk, we present three finite-element formulations for such PDEs, based on H^2-conforming elements[2, 6], the C^0 interior penalty method[1, 5], and a mixed finite-element formulation that explicitly introduces approximations to the gradient of the solution and a Lagrange multiplier[3]. Numerical results highlight the finite-element convergence for all discretizations, and the trade-offs between accuracy and efficiency, particularly for three-dimensional problems.

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High-order embedded finite difference schemes for initial boundary value problems involving mixed derivatives terms in complicated domains

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Key Words: Finite differences, Embedded Finite differences, Initial boundary value problem, parabolic equation, biharmonic equation

Initial Boundary Value Problems (IBVP) arise in many fields, including heat transfer, elasticity, and fluid dynamics. In many cases, the problems' domains have complicated geometries that challenge imposing boundary conditions.

This work presents an approach for designing Bounded-Error Finite-Difference schemes to solve such problems when mixed derivative terms are involved. The general idea is to design a set of modular, one-dimensional operators and find a decomposition of the problem's spatial operator as a linear combination of such operators.

The case of Parabolic IBVP in a two-dimensional domain is analyzed. The limits of this decomposition are found and compared to previously obtained results. The method is then used to construct fourth-order schemes for parabolic IBVP, and the biharmonic equation and simulation results supporting the theory are presented.

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Staggered DG method for the biharmonic problem on polygonal meshes

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Key Words: staggered discontinuous Galerkin, polygonal meshes, error analysis, a posteriori error, biharmonic problems

Recently, we have developed staggered discontinuous Galerkin methods for various problems on general polygonal meshes [1, 2, 3, 4]. In this talk, we present a staggered cell-centered discontinuous Galerkin method for the biharmonic problem with the Steklov boundary condition [5]. Our approach utilizes a first-order system form of the biharmonic problem and can handle fairly general meshes possibly including hanging nodes, which favors adaptive mesh refinement. Optimal order error estimates in L^2 norm can be proved for all the variables. Moreover, the approximation of the primal variable superconverges in L^2 norm to a suitably chosen projection without requiring additional regularity. Residual type error estimators are proposed, which can guide adaptive mesh refinement to deliver optimal convergence rates even for solutions with singularity. Numerical experiments confirm that the optimal convergence rates in L^2 norm can be achieved for all the variables. Moreover, all the provided residual type error estimators show the desired results.

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The Discrete Biharmonic Operator in dimension one: sharp convergence estimates for eigenvalues

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Key Words: *Biharmonic operator, high-order compact scheme, eigenvalues*

The one-dimensional biharmonic operator is a basic model of a high order Sturm–Liouville problem. We study its approximation using a high-order compact discrete biharmonic operator. We find a fundamental connection between this discrete operator and cubic splines, allowing us to derive an explicit expression for the elements of the matrix representing its inverse. Using these results, we prove that the eigenvalues of the discrete operator converge to those of the corresponding continuous problem at an optimal $O(h^4)$ rate.

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Adaptive Data-driven Reduced Order Modelling for Strut-braced Ultra-high Aspect Ratio Wing Configuration

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Key Words: Reduced Order Modelling, Multi-fidelity Aerodynamics, Steady Flows, Transonic Flows

Reduced Order Modelling (ROM) approaches offer promising advantages over CFD simulations in the context of multi-query problems where many high-fidelity simulations must be computed in a repeated manner [1]. For example, in a parametric design and optimisation problem, a huge number of solutions must be obtained describing various geometrical configurations and flight conditions. This reliance on numerical methods is emphasised in the case of new aerodynamic designs where empirical and experimental data is not available. Despite advances in computing, costs can become excessive, especially when the aim is to accurately capture structures in complex three-dimensional flows. This limitation can be overcome by the introduction of ROM techniques that allow for CFD-like accuracy at a fractional cost.

In this work the use of an Adaptive ROM Framework [2] is demonstrated. The framework is adaptive in the sense that a number of ROM methods are used, and their reconstruction error is evaluated. When a new solution is to be computed an automatic selection is performed between the ROMs on the basis of this error metric, so that accuracy is maximised. Since in general no best-in-class method can be identified for a given problem, this approach ensures that for the reconstruction of a particular new solution the most appropriate method is selected. The reduced order methods are coupled with an interpolation technique so that new high-dimensional solutions are recovered non-intrusively. A linear and a nonlinear method will be compared; the latter adopted with the aim to better cope with nonlinear features present in this test-case treated here, e.g. transonic shocks.

Minimising environmental impact is of high interest in the community. To further this goal, aircraft with high-aspect ratio wings offer a promising avenue of development (due to the significant drag reduction) and are identified as a key enabling strategy for sustainable aviation. However, this new design brings additional challenges in terms of aeroelastics. To cope with increased loads and flexibility a strut brace can be introduced as in the configuration presented here. The resulting interference effects lead to additional complexity in the flow further emphasising the advantages of model order reduction.

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Data-driven reduced order models for maternal health

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Key Words: reduced order models, reproductive mechanics, maternal health

Maternal mortality is unacceptably high in many parts of the world, with 810 women dying each day due to complications of pregnancy and childbirth. Moreover, many mothers who survive pregnancy and childbirth suffer from lifetime morbidity, disabilities and ill-health. Though the causes of pregnancy-related death and illness are various, mechanical and structural changes of the reproductive organs contribute to their development. Currently, there are no science-based tools that can predict trauma during childbirth. Once the mother is in labor, the obstetrician has very limited time to evaluate the best course of action for delivery, including a C-section.

While recent advances in childbirth finite element (FE) simulations have quantified damage to the pelvic organs and tissues, the complexity of such simulations (geometry, boundary conditions, nonlinear materials, etc.) results in long run-times yielding an impractical resource for obstetricians. Reduced order modeling (ROM) is a mathematical numerical approach capable of solving very complex simulations with significant time-savings. In this study, we propose the use of the Galerkin projection-based ROM to describe the mechanical response of vaginal tissue in *ex vivo* mechanical tests as a first step towards implementing ROM for childbirth simulations. Efficient and accurate simulations of the pelvic organs and tissues could help save the lives of mothers and address preventable maternal morbidity and disabilities by providing science-based descriptive and predictive tools that can be used by obstetricians.

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Geometric Structure-Preserving Design Space Dimensionality Reduction

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Key Words: Geometric moments, Dimensionality reduction, Shape optimisation, Parametric design

Shape optimisation problems often suffer from the curse of dimensionality: the computational complexity rises exponentially with the dimension of a design space [1]. One approach to cure this issue is to exploit the latent features, which forms a reduced dimensional subspace. The commonly used approaches, such as principal component analysis (PCA) [2], usually generate subspaces that often fail to accommodate physical information and preserve the intrinsic geometric structure of the shape, thus resulting in many invalid geometries.

In this work, we propose a Shape-Signature Subspace (SSS) technique for dimension reduction, which uses higher-level information about the shape in terms of its geometric integral properties. In our case, these integral properties are geometric moments [3] of varying order. Their usage is based on the fact that moments of a shape are intrinsic features of the shape's geometry, and they provide a unifying medium between geometry and physics. To maximise the geometric information retained in the subspace, we evaluate a set of composite moments, using the divergence theorem, for disintegrated sub-geometries of the shape. These moments are used with the shape modification function to form a shape signature vector (SSV), which act as a descriptor to uniquely represent each design in the design space. Afterwards, we use SSV to perform eigendecomposition, which results in spanning the basis of a subspace retaining the highest variance in terms of geometry, its underlying structure and physics.

The feasibility of the proposed method is tested for optimising a ship hull, parameterised with 27 design parameters, against its wave resistance coefficient (c_w). The results showed that subspace obtained with PCA results in 44% of reduction in the original design space dimensionality, whereas 70% of dimension reduction is achieved with SSS. The number of invalid geometries produced by the SSS-based subspace is 36% less with faster to the optimal solution compared to the subspace formed with PCA.

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Improved gradient enhanced Kriging model for high-dimensional function approximation

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Key Words: Gradient-enhanced Kriging, global sensitivity analysis, hyper-parameter optimization

The statistical interpolation method Kriging, also known as Gaussian process regression, has been widely used to construct surrogates for approximating expensive computational models in various disciplines. However, the training sample size required to construct an accurate Kriging model rises rapidly with the input dimension. The gradient-enhanced Kriging (GE-Kriging) model has the potential to alleviate this problem known as the ”curse of dimensionality” by incorporating gradient information. However, GE-Kriging tends to get impractical for high-dimensional problems due to the large correlation matrix and the associated time-consuming hyper-parameters tuning procedure.

To address these issues, in this talk, an improved GE-Kriging model is proposed, reducing both the correlation matrix size and the number of hyper-parameters. This is achieved by performing a derivative-based global sensitivity analysis to detect a subspace within which the model response exhibits strong variability. The correlation matrix of GE-Kriging, in turn, is reduced by incorporating partial derivatives only within the identified subspace. Additionally, we transform the original high-dimensional hyper-parameter tuning problem into a low-dimensional counterpart by learning the relationship between the model hyper-parameters and the global sensitivity indices. The proposed method is validated with several benchmark problems of various dimension. The results show that the proposed GE-Kriging model features an accuracy that is comparable to the traditional one but comes with much less training costs, which makes it more practical for applications involving high-dimensional problems. Eventually, it is planned to employ this method in surrogate modeling-assisted process and energy optimization in the context of car body painting.

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LEAST-ORDER MODELS BASED ON THE FLOW INSTABILITIES

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Key Words: Fluid Dynamics, Reduced-Order Model, Bifurcations, Nonlinear Dynamics.

Fluid flows obey the Navier-Stokes equations, which are nonlinear partial derivative equations and make such dynamical systems of infinite dimension. Yet, the dynamical systems usually evolve on inertial manifolds of finite dimensions. Identifying the elementary degrees of freedom is highly desirable and challenging to construct meaningful reduced-order models (ROMs) for human understanding, dynamic prediction and control. Galerkin methods, commonly used to produce ROMs, neither tell how many modes should be considered, nor which modes should be considered. The least-order model based on the flow instabilities is addressed in the case of the fluidic pinball, a two-dimensional flow configuration consisting of three discs at the vertices of an equilateral triangle in the cross flow.

In this system, the steady solution undergoes a supercritical Hopf bifurcation at $Re_{HP} \approx 20$, resulting in the formation of a von Kármán street of vortices. Beyond $Re_{PF} \approx 70$, the system undergoes a secondary supercritical pitchfork bifurcation with the appearance of two additional mirror-conjugated (unstable) steady solutions, which break the reflectional symmetry of the configuration by twisting the jet behind the two downstream cylinders. Based on the normal forms of the two bifurcations, the ROM must be at least five dimensional, three degrees of freedom being associated with the Hopf bifurcation, two with the pitchfork bifurcation [1]. The coefficients of the model are determined partly by the physical inspection of the transient and post-transient dynamics, partly by the sparse identification with the SINDy algorithm under constraints [2]. This modelling strategy with sparse calibration embeds physical knowledge into Galerkin models, which is also applied to build a force-oriented ROM [3].

With only five degrees of freedom, the ROM reliably reproduces the dynamics of the fluidic pinball from the initial condition to the post-transient regime, including 3 steady and 3 periodic solutions. This ROM serves as example for similar flow dynamics and as a benchmark for future fully automated reduced-order modeling methods.

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Model Reduction of Convection-Dominated Partial Differential Equations via Optimization-Based Implicit Feature Tracking

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Key Words: Shock Fitting, Discontinuous Galerkin, PDE-Constrained Optimization

Reference link: https://www.wccm2022.org/submission.html

This work introduces a new approach to reduce the computational cost of solving partial differential equa- tions (PDEs) with convection-dominated solutions: model reduction with implicit feature tracking. Traditional model reduction techniques use an affine subspace to reduce the dimensionality of the solution manifold and, as a result, yield limited reduction and require extensive training due to the slowly decaying Kolmogorov n-width of convection-dominated problems. The proposed approach circumvents the slowly decaying n-width limitation by using a nonlinear approximation manifold systematically defined by composing a low-dimensional affine space with a space of bijections of the underlying domain. Central to the implicit feature tracking approach is a residual minimization problem over the reduced nonlinear manifold that simultaneously determines the reduced coordinates in the affine space and the domain mapping that minimizes the residual of the unreduced PDE discretization. This is analogous to standard minimum-residual reduced-order models, except instead of only minimizing the residual over the affine subspace of PDE states, our method enriches the optimization space to also include admissible domain mappings. The nonlinear trial manifold is constructed by using the proposed residual minimization formulation to determine domain mappings that cause parametrized features to align in a reference domain for a set of training parameters. Because the feature is stationary in the reference domain, i.e., the convective nature of solution removed, the snapshots are effectively compressed to define an affine subspace. The space of domain mappings, originally constructed using high-order finite elements, are also compressed in a way that ensures the boundaries of the original domain are maintained. Several numerical experiments are provided, including transonic and supersonic, inviscid, compressible flows, to demonstrate the potential of the method to yield accurate approximations to convection-dominated problems with limited training.

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NONLINEAR MANIFOLD TO COMPONENT-WISE REDUCED ORDER MODELS TOWARDS MULTI-SCALE PROBLEMS

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Key Words: *reduced order model, multi-scale problems, data-driven physical simulation*

Traditional linear subspace reduced order models (LS-ROMs) can accelerate physical simulations in which the intrinsic solution space falls into a subspace with a small dimension, i.e., the solution space has a small Kolmogorov n-width with a small n. However, for physical phenomena not of this type, e.g., any advection-dominated flow phenomena such as in traffic flow, atmospheric flows, and air flow over vehicles, there is no linear subspace that approximates the solution well with a small dimension. Furthermore, high-dimensional parameter space poses a serious issue of computationally expensive training cost due to the number of training data increasing exponentially with the parameter space dimension. To address cases such as these, I will present two different reduced order model techniques.

The first one is a fast and accurate nonlinear manifold ROM (NM-ROM) [1] that can better approximate high-fidelity model solutions with a smaller latent space dimension than the LS-ROMs. Numerical results show that neural networks can learn a more efficient latent space representation on advection-dominated data from 1D and 2D Burgers' equations. Speedup of 10x and relative error of less than 1% are achieved with an appropriate treatment of the nonlinear terms through a hyper-reduction technique.

The second one is a component-wise reduced order model (CW-ROM) [2] that resolves the challenge posed by a high-dimensional parameter space. The CW-ROM enables a smaller size and parameter set of training, resulting in an efficient training procedure. Furthermore, the accuracy can be tuned, so an arbitrarily accurate solution can be achieved with a considerable speedup. It is applied to a multi-scale topology optimization problem, i.e., lattice-type structure design optimization, achieving a speed-up of 1000x with a relative error less than 1%.

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Reduced Order Modeling for a LES filtering approach

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Key Words: Proper orthogonal decomposition, Reduced order model, Large Eddy Simulation, filter stabilization, projection-based methods, data-driven strategies

It is well known that the extension of reduced order models (ROMs) to turbulent flows presents several challenges. We choose to work with a large eddy simulation (LES) approach that describes the small-scale effects by a set of equations to be added to the discrete Navier-Stokes equations [1]. This extra problem acts as a low-pass differential filter. We propose a Proper Orthogonal Decomposition (POD)-Galerkin based ROM when a linear filter is used [2] and a hybrid projection/data-driven strategy in the case of a nonlinear filter [3]. The novelties of our ROMs include: 1) the use of a ROM differential filter, i.e. a ROM spatial filter that uses an explicit lengthscale, 2) the computation of the pressure field at the ROM level, 3) the use of a finite volume method for the space discretization, which is common in many commercial codes, and 4) the use of different POD coefficients and bases to approximate the intermediate and end-of-step velocities. The performance of the proposed methods is assessed through 2D and 3D test cases.

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A C^0 FINITE ELEMENT METHOD FOR THE BIHARMONIC PROBLEM WITH NAVIER BOUNDARY CONDITIONS

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Abstract. We study the biharmonic equation with the Navier boundary conditions in a polygonal domain. In particular, we propose a method that effectively decouples the 4th-order problem into a system of Poisson equations. Different from the usual mixed method that leads to two Poisson problems but only applies to convex domains, the proposed decomposition involves a third Poisson equation to confine the solution in the correct function space, and therefore can be used in both convex and non-convex domains. A C^0 finite element algorithm is in turn proposed to solve the resulted system. In addition, we derive the optimal error estimates for the numerical solution on both quasi-uniform meshes and graded meshes. Numerical test results are presented to justify the theoretical findings.

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A New Framework for the Stability Analysis of Perturbed Saddle-point Problems and Applications

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Key Words: *Fitted Norms, Stability Analysis, Saddle-point Problems, LBB Condition, Poromechanics, Biot's Model.*

This talk provides a new abstract stability result for perturbed saddle-point problems which is based on a proper norm fitting. We derive the stability condition according to Bauska's theory from a small inf-sup condition, similar to the famous Ladyzhenskaya-Bauska-Brezzi (LBB) condition, and the other standard assumptions in Brezzi's theory under the resulting combined norm. The proposed framework allows to split the norms into proper seminorms and not only results in simpler (shorter) proofs of many stability results but also guides the construction of parameter robust norm-equivalent preconditioners. These benefits are demonstrated with several examples arising from different formulations of Biot's model of consolidation.

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Least squares discretization and preconditioning for singularly perturbed problems

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Key Words: Least squares, Saddle Point Systems, Mixed Methods, Optimal Test Norm

We consider a least squares method for discretizing singularly perturbed second order elliptic problems. Choices for discrete stable spaces are considered for the mixed formulation and a preconditioned conjugate gradient iterative process for solving the saddle point reformulation is proposed. We provide a preconditioning strategy that can be applied to a large range class of mixed variaional formultations. Using the concepts of optimal test norm and saddle point reformulation we provide a robust discretization strategy that works for uniform and non-uniform refinements for Convection-Reaction-Diffusion problems.

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Monolithic Multigrid for a Reduced-Quadrature Discretization of Poroelasticity

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Key Words: Poroelasticity; Reduced Quadrature; Finite Elements; Monolithic Multigrid; Local Fourier Analysis

Advanced finite-element discretizations and preconditioners for models of poroelasticity have attracted significant attention in recent years. The equations of poroelasticity offer significant challenges in both areas, due to the potentially strong coupling between unknowns in the system, saddle-point structure, and the need to account for wide ranges of parameter values, including limiting behavior such as incompressible elasticity. The work presented in this talk was motivated by an attempt to develop monolithic multigrid preconditioners for a novel P1-P0-RT-stabilized discretization; we show here why this is a difficult task and, as a result, we modify the discretization through the use of a reduced quadrature approximation, yielding a more "solver-friendly" discretization. Local Fourier analysis is used to optimize parameters in the resulting monolithic multigrid method, allowing a fair comparison between the performance and costs of methods based on Vanka and Braess-Sarazin relaxation. Numerical results are presented to validate the LFA predictions and demonstrate efficiency of the algorithms. Finally, a comparison to existing block-factorization preconditioners is also given.

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On the Necessity of the Inf-Sup Condition for a Mixed Formulation

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Key Words: Inf-sup condition, Finite elements, Poisson problem, Stability and convergence

It is well known that stable approximations of mixed problems rely on suitable inf-sup conditions [1]. Usually, non stable formulations are considered dangerous and people prefer to avoid them unless suitable stabilizations are used.

We consider a non-conventional mixed approximation of the Poisson problem for which the inf-sup constant is not uniformly bounded as the mesh is refined [2].

The behavior of the inf-sup condition is discussed and the convergence of the finite element approximation is studied. It turns out that, under appropriate hypotheses on the data, the discrete solution is stable and optimally convergent.

Several numerical tests confirm the theoretical results and shed some light on the links between the inf-sup condition and the convergence of the discrete solution.

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Saddle Point Least Squares for Convection-Diffusion

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Key Words: Saddle Point Least Squares, Preconditioning, Mixed Methods

We consider a Saddle Point Lease Squares reformulation for the discretization of the Convection-Diffusion. A focus is placed in the convection dominated regime which is known to produce non-physical oscillations. We consider also streamline diffusion stabilization to remedy the oscillatory behavior. For the choice of stable pairs of spaces, we are able to equipt these spaces with an intentional choice of inner products to allow for the use of precondioners from Reaction-Diffusion equations. We couple this with the concept of optimal test norms to provide an efficient discretization strategy.

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A Comparison of Three Iterative Solution Schemes for Elliptic PDEs

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Finite element and discontinuous Galerkin discretizations of linear elliptic PDEs require the solution of global systems of linear equations. The size of the stiffness matrix quickly increases with the number of elements, as does the condition number in certain cases. These properties pose serious challenges in the direct solution of elliptic PDEs. We investigate three iterative solution schemes for two classes of elliptic problems: those that arise as the steady-state limits of parabolic or hyperbolic PDEs and those that represent long-term solutions of hyperbolic PDEs driven by harmonic forces, in particular, the Helmholtz equation.

The first two schemes use a hyperbolic PDE solver, the causal Spacetime Discontinuous Galerkin (cSDG) method [1], to solve indirectly the underlying elliptic PDE. The cSDG method is very effective in this role due to its local conservation properties, linear computational complexity, unconditional stability, powerful space-time adaptive meshing capabilities, and other favorable properties. In the first scheme, applicable only to steady-state limit problems, we solve a damped hyperbolic PDE over a sufficiently long time interval to find its solution's steady-state limit. We tune viscous damping [2] or kinetic damping [3] parameters to accelerate solution convergence. In the second scheme, applicable to both classes of elliptic PDEs under consideration, we seek initial conditions for substitute hyperbolic problems that satisfy conditions specific to each elliptic problem class. The solution to the target elliptic PDE is obtained by applying certain projection operators to the hyperbolic solution for the converged initial condition. This method resembles the *WaveHoltz* method [4] for the Helmoltz equation. We propose a new method for steady-state limit problems based on matrix-free iterative linear system solvers such as GMRES. The third scheme does not involve a hyperbolic solution. We instead apply asynchronous aspects of the cSDG algorithm to develop a new indirect solver for elliptic problems in which we solve a series of localized elliptic problems until the global residual is sufficiently small. The localized solutions are ordered by the current local residual magnitudes, rather than a predefined geometric pattern as in Gauss-Seidel methods, and can be performed asynchronously in parallel.We compare the performance of the three solution schemes in terms of their accuracy and computational efficiency.

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A coupled-mode theory for exterior scattering problems based on a non-orthogonal modal expansion

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Key Words: *Coupled-mode theory, scattering analysis, exterior problem, Helmholtz equation*

This study presents a novel numerical method for exterior scattering problems. The proposed method is based on a coupled-mode approach, which formulates the scattering process in terms of resonance and radiation.

To this end, we separate an entire unbounded space into a ball (disk) and its exterior. The fictitious ball contains all inhomogeneity (scatterer); therefore, the exterior is homogeneous and supports cylindrical/spherical waves with a continuous spectrum. To represent a resonant field in the vicinity of a scatterer, we expand a scattered field in terms of normal modes in the ball with a discrete spectrum.

Unlike quasinormal mode expansion [1], the normal modes form a complete set in the ball when a suitable boundary condition is imposed on its surface. Although the most common choice for this auxiliary condition is the Neumann boundary condition [2], we suffer from severely slow convergence of the Neumann modal expansion due to a nonzero Neumann data on the surface.

In this study, we propose a rapidly convergent expansion for the resonant field. The proposed expansion is comprised of both the Neumann and Dirichlet eigenfunctions in the ball. Since the L2 orthogonality does not hold between Neumann and Dirichlet eigenfunctions, the proposed expansion is non-orthogonal. We perform some numerical verifications of the proposed method and demonstrate its effectiveness.

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A Parallel–Adaptive Spacetime Discontinuous Galerkin Solver for Three-Dimensional Hyperbolic Systems

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Key Words: Spacetime, Parallel, Adaptive Meshing, Discontinuous Galerkin, Hyperbolic PDEs

The causal Spacetime Discontinuous Galerkin (cSDG) method is a powerful scheme for solving hyperbolic systems of PDEs that features local conservation properties, linear computational complexity, unconditional stability for linear problems, powerful space-time adaptive meshing capabilities, and other favorable properties. The method has been applied to elastodynamics and stochastic brittle fracture [1, 2] as well as contact, conservation laws, electromagnetics, hyperbolic conduction and advection–diffusion. In lieu of synchronous time marching, it constructs unstructured spacetime meshes according to a causality constraint that localizes the solution process to small clusters of spacetime elements called patches [3]. The solution on each patch depends only on adjacent, previously-solved elements and prescribed initial and boundary data. This structure supports efficient patch-by-patch solution procedures.

This presentation introduces a new generation of cSDG software called *ParaSDG* that incorporates recent advances in parallel implementations of the cSDG method on distributed HPC platforms as well as adaptive spacetime meshing technologies in up to three spatial dimensions and time. The asynchronous distributed implementation features a fine-grained patch-wise parallel architecture in lieu of traditional domain decomposition and novel stochastic procedures for balancing distributed data storage and computational load. Nearly the entire algorithm, including spacetime patch generation, localized cSDG solution procedure, and adaptive meshing operations, is embarassingly parallel and executed in local process-private memory. ParaSDG's spacetime meshing extends adaptive causal meshing up to three spatial dimensions with a new adaptive refinement algorithm and the use of harmonic triangulation procedures. Numerical examples will demonstrate ParaSDG's capabilities and parallel performance.

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An adaptive nonlinear elimination preconditioned space-time solution algorithm for hyperbolic partial differential equation problems

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Key Words: Fully-coupled space time algorithm, Hyperbolic partial differential equations, shock wave, Nonlinear elimination preconditioning, Inexact Newton method

As the computing power of the latest parallel computer systems increases dramatically, the fully coupled space-time solution algorithms for the time-dependent PDEs obtained their popularity recently for temporal domain parallelism. This space-time algorithm solves the resulting large, space, nonlinear systems in an all-at-once manner. A robust and efficient nonlinear solver plays an essential role as a critical kernel of the whole solution algorithm. This talk introduces some nonlinear preconditioned Newton algorithms for the space-time formulation of Burgers' equation with shock presented. In that case, the history of the nonlinear residual norm for the classical Newton method suffers from a long stagnation period due to strong local nonlinearity. To overcome the difficulties, we apply an adaptive nonlinear elimination preconditioning technique to enhance the robustness of the inexact Newton method, in the sense that the number of inexact Newton iterations required to converge is almost independent of both of the time-step and the mesh sizes. Some numerical results show that the proposed method is more robust and efficient than the commonly-used classical inexact Newton algorithm.

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Implicit Trefftz discontinuous Galerkin method

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Key Words: discontinuous Galerkin method, Trefftz method

We present a novel numerical method to reduce the discrete system size of discontinuous Galerkin (DG) methods, inspired by Trefftz methods. The main idea of Trefftz methods, originating from [1], is to choose optimal discretization spaces to reduce the number of unknowns. This usually requires the construction of specific test and trial functions that need to be tailored to the PDE in question. These approaches pair well with DG methods so that the basis construction of elements decouples.

The starting point for the approach presented here, will be a suitable DG scheme with polynomial test and trial functions. The knowledge of the Trefftz function space is then injected implicitly by finding a *Trefftz embedding* that maps the Trefftz space into the discretization space. Thus no basis for the Trefftz space has to be calculated, which makes it possible to apply this approach even if a basis for the Trefftz space is unknown. The embedding then allows to significantly reduce the size of the finite element matrix, allowing for faster solving times.

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Space-Time Embedded-Hybridized Discontinuous Galerkin Method for Fluid-Rigid Body Interaction Problems

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Key Words: Space-Time, Hybridizable Discontinuous Galerkin, Fluid-Rigid Body Interaction

Fluid-rigid body interactions are often encountered in real-world applications, such as airflow around turbines, bridges, or tall antennas. In this talk, we present a Space-Time Embedded-Hybridized Discontinuous Galerkin method to solve the fluid subproblem that allows for an arbitrarily high order approximation in space and time. The rotation and the translation of the rigid body are described by ordinary differential equations, which are coupled to the fluid problem via the pitching and the lifting forces. We introduce a sliding grid technique for the rotational movement that can handle arbitrary rotation. The numerical examples will include galloping and fluttering motion.

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Symplectic Hamiltonian finite element methods for electromagnetics

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Key Words: time-dependent Maxwell's equations, symplectic Hamiltonian finite element methods, mixed methods, discontinuous Gakerkin methods, hybridizable discontinuous Galerkin methods

We present a general approach for defining high-order accurate finite element methods for the Maxwell's equations which provide time-invariant, non-drifting approximations to the total electric and magnetic charges, and to the total energy. We devise these methods by taking advantage of two of the Hamiltonian structures of the Maxwell's equations. The first is based on the standard formulation of the equations in terms of the electric and magnetic fields, whereas the second is based on a wave-like rewriting of them in terms of the electric and the magnetic potential fields. For each of these Hamiltonian structures, we proceed as follows. First, we introduce spatial discretizations of the Maxwell's equations using mixed finite element, discontinuous Galerkin, and hybridizable discontinuous Galerkin methods to obtain a semi-discrete system of equations which display discrete versions of the Hamiltonian structure of the Maxwell's equations. Then we discretize the resulting semi-discrete system in time by using a symplectic integrator. This ensures the conservation properties of the fully discrete system of equations. There is a Symplectic DG method for the first formulation [J. Sci. Comput. 35, pp. 241–265, 2008] but all other methods are new. We show that there are no Symplectic HDG methods for the first formulation. In contrast, we devise Symplectic Hamiltonian mixed, DG, and HDG methods for the second formulation. Finally, for the Symplectic HDG method, we present numerical experiments which confirm its optimal orders of convergence for all variables and its conservation properties for the total linear and angular momenta, as well as the total energy. Finally, we discuss the extension of our results to other boundary conditions and to numerical schemes defined by different weak formulations.

Benchmarking the Regridding Functionality of Climate Modelling Coupling Software

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Key Words: *Regridding, Remapping, Interpolation, Code Coupling, Climate Modelling,*

We present here the results of a benchmarking exercise performed on the SCRIP library [1], ATLAS [2], MOAB-TempestRemap [3], YAC [4], ESMF [5] and XIOS [6]. The motivation is to complement the SCRIP library regridding algorithms implemented in the OASIS3-MCT coupler.

In order to compare these libraries, several aspects had to be covered. In a preliminary analysis, we first enquired about available regridding methods and evaluated the software development environment, e.g. the coding language, project history and development plans, provision of support to external projects, and committed manpower.

Then we proceeded to a formal benchmarking of SCRIP, YAC, ESMF and XIOS. 5 regridding algorithms (nearest-neighbour, bilinear, bicubic, 1st and 2nd order conservative remapping) were evaluated with 4 different functions, some of them having strong gradients, for 14 couples of grids used in real ocean or atmosphere models. Metrics proposed by the CANGA project (https://github.com/CANGA/Remapping-Intercomparison) quantifying the sensitivity, conservation, consistency, monotonicity, and performances of the library were calculated.

After interactions with the library developers to solve specific issues, it is concluded that YAC, ESMF and XIOS show very good results for the regridding algorithm, functions and grids evaluated. A unified scripting environment for SCRIP, ESMF and XIOS is now available in the latest version of the OASIS3-MCT coupler so that users can test those three libraries on their own grid for their own regriddings. Detailed results of this benchmarking exercise are available in [7]

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Efficient Multi-Material Remap in High-Order ALE Hydrodynamics

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Key Words: Remap, ALE Hydrodynamics, High-Order Finite Elements, Matrix-Free Methods

We present a remap algorithm in the context of multi-material Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics discretized with high-order finite elements [1]. The major mathematical challenges for this system include (i) conservation of the per-material volumes, masses, and energies, (ii) preservation of the minimum and maximum local bounds for all primary fields (e.g. density), which requires per-material synchronization between conserved fields (e.g. the ratio of mass and volume), (iii) synchronization between all material volume fractions, i.e., they must sum to unity at all degrees of freedom, and (iv) minimization of numerical diffusion and spreading of small volume fractions due to the nature of the finite element approach. We will discuss our latest methods for addressing the above challenges and demostrate them on standard ALE hydrodynamics benchmarks.

When high-order finite elements are used, the main limitation in terms of efficiency is the use of classical assembly and global sparse matrices. These scale poorly as the order of the finite element discretization increases and involve expensive data motion which is undesirable for the newest computer architectures. We will discuss our recently developed matrix-free remap formulation based on partial assembly [2] and demonstrate its performance benefits for practical ALE simulations.

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Evaluation of Radial-Basis-Function Data Mappings of the Coupling Library preCICE

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Key Words: Multi-physics, Radial Basis Function, Coupled Simulation

In partitioned multi-physics simulation, multiple solvers interact together along a common coupling interface. This approach requires spatial data mapping methods, as each subsystem is discretized separately with potentially non-matching meshes at the common coupling interface. Radial-basis-function (RBF) mappings employ radially symmetric functions on an input mesh to perform the mapping to an output mesh [2]. We have implemented various mapping variants in the black-box coupling library preCICE [1]. In this work, we compare different RBF mappings with projection-based mapping methods.

In preCICE, the implementation of the RBF mapping method relies on PETSc as a parallel linear algebra solver [3]. We test the implementation in terms of efficiency as well as accuracy using a wind turbine blade geometry, a realistic geometry in practical applications. Results show that only for the coarsest meshes one can apply global basis functions due to the large memory storage requirements as well as the high computational complexity. Compact basis functions with a local support radius are able to provide accurate interpolation, while utilizing less memory space and being computationally cheaper. Projection-based interpolation methods can be implemented in a more efficient way compared to RBF mapping methods. However, the resulting mapping is typically less accurate or violates a strict black-box coupling approach operating solely on a point-cloud.

We further give an outlook on three current and future data mapping extension in preCICE: as a first variant, we introduce an in-solver mapping method, where the interface vertices of each solver are shared, and each solver directly performs the mapping request based on its own discretization. As a second variant, we investigate a RBF partition of unity method that is suitable for scalable data interpolation with minimal parallel communication. The third variant employs a nearest-neighbor mapping with additional gradient data in order to improve the accuracy of the plain nearest-neighbor mapping.

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Remapping native fields for climate applications

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Key Words: *native field transfer, generalized moving least squares, CANGA*

Coupling global Earth system models requires passing information between sub-models that have been discretized independently and may employ different types of native field representations on different types of meshes. In E3SM's MPAS-Ocean, for example, velocities are represented with Raviart-Thomas basis elements on simplices and must be remapped to nodal spectral elements on hexahedral grids discretizing the domain for the atmosphere.

Generalized moving least squares (GMLS) is a non-parametric regression framework able to construct approximations to fields from scattered data. Judicious selection of sampling functionals and target functional for GMLS makes it is possible to approximate the embedded continuous functions represented by coefficients to a native field basis, e.g. Raviart-Thomas, Nedelec, or cell-averaged. This flexibility in GMLS makes it a prime candidate for general purpose coupling applications.

Remap over a sphere is performed by first approximating the tangent plane for each point where a field reconstruction is requested. The tangent plane approximation is then used as a local coordinate system on which sampling functionals are evaluated acting on a basis. After solving a local least squares problem, the field is then reconstructed in the local coordinate system, and transformed to the global coordinate system, if necessary.

The Compadre toolkit is used for the implementation of all described techniques. Numerical results will be presented demonstrating the accuracy of remap of several fields on grids where the degrees of freedom represent cell-averaged quantities and face normal averages (Raviart-Thomas).

Disclaimer. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. SAND2021-14460 A.

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WLS-ENO Remap for Cell-Averaged Data and Anisotropic Meshes on Surfaces

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Key Words: weighted least squares; data transfer; remap; cell-averaged data; superconvergence; discontinuities; Gibbs phenomenon; essentially non-oscillatory schemes

In multiphysics simulations, data are often transferred between different meshes at high-order accuracy. Jumps or discontinuities in the data or highly anisotropic meshes can pose significant challenges in data remap. In this work, we extend our earlier work on WLS-ENO Remap [2] for remapping node-based data to support cell-averaged data, such as those arising from finite-volume methods, including remapping between cell-averaged and node-based data. Based on the Weighted-Least-Squares-based Essentially Non-Oscillatory (WSL-ENO) schemes [1], WLS-ENO Remap achieves superconvergence when remapping smooth functions while overcoming overshoots and undershoots (aka Gibbs phenomena) for discontinuous functions. In addition, we introduce adaptive quadrature and adaptive stencils to overcome the potential loss of accuracy or conservation due to highly discrepant meshes or highly anisotropic meshes, such as those near the south and north poles of a longitude-latitude mesh of a sphere. We compare our technique with a conservative high-order remap to transfer functions on spheres. We show that our proposed technique is competitive in accuracy and conservation, despite not using a common-refinement mesh while being more flexible and easier to implement and more robust against discontinuities, anisotropic meshes, and rounding errors.

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An adaptive scheme for free-surface seepage problems in porous media

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Key Words: Seepage problem, tailing dam, numerical stabilization, adaptive refinement

Seepage problems with free surfaces have been a matter of interest in engineering and mathematics due to the strong non-linearities involved. The significant difference in densities between the air and the water restricts the flow domain, producing a free surface. However, finding its exact location is still a challenge. Several numerical techniques are used to solve this phenomenon; nevertheless, some of these methods suffer from some instabilities when sharp changes in permeability occur if the mesh in the interface is not well defined, leading to unphysical oscillations in the numerical outputs.

Recently, a novel adaptive stabilized finite element method for linear problems is described in [1]. This method combines the residual minimization idea and the stability provided by the discontinuous Galerkin method approach. This leads to obtaining a stable continuous solution from the classical FEM and a residual representative that helps to develop mesh refinement adaptivity.

This project is divided into two parts: First, we discuss some numerical aspects of a non-linear adaptive approach for tailing dam application. Then, we implement the aforementioned numerical framework to find the correct position of the free surface scheme through an automatic adaptive procedure by using a solution-dependant permeability coefficient.

As a result, the residual estimative leads to obtaining a stable representation of the free surface and reducing the computational effort required by other approaches.

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Scale Bridging Dislocation Networks with Length Distributions

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Key Words: *Dislocation, Plasticity, Scale Bridging*

Scale bridging from discrete defects to continuum field descriptions is always a fundamental challenge in theory development. In the case of dislocation-mediated plasticity, the challenge is to identify a suitable coarse-grained descriptor of the dislocation network which still retains enough physics so that information obtained from discrete dislocation models can be folded into the coarse-grained governing equations [1]. We propose using dislocation length distributions as a coarse-grained descriptor for the network [2], coupled with discrete dislocation dynamics (DDD) simulations aimed at characterizing evolution behaviors of the network. This concept builds on a theory developed by Ardell and colleagues which has disappeared into the literature [3]. In this talk, we demonstrate the concept underlying our scale bridging framework along with preliminary results on its development. Specifically, we show how careful analysis of DDD simulations provides insights into junction formation and dissolution, plastic strain rate, and dislocation multiplication which serves as direct input into the coarse-grained model. Our approach provides a viable pathway towards constructing non-phenomenological models for plasticity.

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A boundary element method for evaluating high-order frequency derivatives of acoustic wave scattering by periodic structures

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Key Words: Fast frequency sweep, Acoustic scattering, Periodic structure, Boundary element method, Automatic differentiation, Ewald method

Emerging acoustic metamaterial and metasurface, as well as some existing acoustic structures such as sound-proofing walls, may often have periodic geometry. They exploit some resonance and interference peculiar to the periodic structures to manipulate sound waves. The anomalous behaviours can, however, be observed only if the excitation frequency is very close to the eigenfrequency unique to each structure, which may lead to the narrow working band of the structure. In practical use, more or less frequency fluctuation is expected, and the working band should be wide to some extent. We thus are motivated to develop a structural optimisation for the periodic acoustic structures with wide working bandwidth.

In recent years, various structural optimisation for acoustic design are reported. Some researchers have already addressed optimal design methods for wideband acoustic devices. Such attempts can be classified into two types; One is based on robust topology optimisation [1, 2], while the other defines the objective function as the frequency-averaged scattering response [3, 4]. In both methods, the frequency response of the amplitude is estimated with the Taylor series or the Padé approximation based on its frequency derivatives. We have reported that the boundary element method combined with the automatic differentiation [2, 4] would be an ideal choice to compute the derivatives especially when the underlying boundary value problem is defined in an exterior domain.

In the present talk, we shall extend the boundary element method with the automatic differentiation to the periodic scattering problem. The boundary integral equation for the sound pressure is formulated with the Green function that satisfies the quasi-periodic boundary condition, whose frequency derivatives give the integral equations of the derivatives of the pressure. The kernels of the differentiated integral equations thus obtained are the frequency derivatives of the Green function. We develop a numerical method based on the Ewald method and the automatic differentiation to compute the kernels. We further implement the boundary element method based on the present kernel computation method. In the talk, we shall present some validation results and discuss the future directions.

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A preconditioner based on Calderón's formulae for isogeometric boundary element methods for Maxwell's equations

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Key Words: BEM, Isogeometric analysis, Collocation, Calderón's preconditioner

The Calderón preconditioner for the isogeometric BEM (boundary element method) discretised with the collocation for Maxwell's equations is investigated in this paper. The Calderón preconditioning for the EFIE with the Galerkin method in general requires the use of the dual basis function such as the Buffa-Christiansen basis functions, which causes much computational time. We show that a dual basis function in the isogeometric BEM can be introduced in the same way as the original basis function, and that the computational time of a matrix corresponding to the EFIO (Electric field integral operator) discretised with the dual basis function is as much as that with the original basis function. With some numerical examples, we verify that matrices preconditioned with the proposed method are well-conditioned.

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An acceleration of the time-domain boundary element method for electromagnetic scattering problems in 3D

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Key Words: Time-domain Boundary Element Method, Fast Multipole Method, Electromagnetics

The purpose of this study is to establish a fast and memory-efficient time-domain boundary element method (TDBEM) for 3D transient electromagnetic wave problems on the basis of our previous study for the 3D wave equation [1, 2]. In the previous study, we developed a fast algorithm that is a variant of the fast multipole method (FMM) [3] and exploits the interpolation of the fundamental solution (and its derivatives). Similarly, we will show that an interpolation-based FMM can be formulated for the 3D Maxwell equations by considering, in particular, the Rao–Wilton–Glisson basis [4] and its analytical integrals. The computational complexity of the resulting fast (and approximating) TDBEM can be theoretically estimated as $O(N_{\mathrm{s}}^{\delta} N_{\mathrm{t}})$, where N_{s} and N_{t} denote the number of boundary elements and time-steps, respectively, and the exponent δ is $4/3$ or $3/2$ according to the assumption of the distribution of the boundary elements in space [1]. This is essentially faster than the conventional TDBEM with the complexity of $O(N_{\mathrm{s}}^2 N_{\mathrm{t}})$. As well as the conventional method, the fast method can deal with the models (scatterers) in arbitrary shapes in free (unbounded) space. Therefore, it can outperform the finite-difference time-domain (FDTD) method, which is the standard numerical method for the unsteady electromagnetic problems.

In this talk, we will formulate the interpolation-based FMM for 3D electromagnetic and show some numerical examples to validate the formulation.

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Boundary element method to investigate the interaction between geometrically necessary dislocations and voids by the nonsingular dislocation theory

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Key Words: *Boundary element method, Nonsingular dislocation theory, Dislocation loop, Void, Image stress*

Dislocations are known as line defects in metallic materials, whose formation and movement dictates the plastic deformation. Geometrically necessary dislocations are the ones to accommodate for the deformation in a crystalline material. In an infinite elastic solid, the stress field generated by a dislocation can be obtained using Green's function, which resulted in either a surface integral for unclosed dislocation curves or a contour integral for a general dislocation loop [1]. Interestingly, this methodology shares similarity with that of the boundary element method. More recently, the modification that contributed to the removal of singularity in the stress field near the dislocation core eases the usage of the formula [2]. In particular, the nonsingular dislocation integral is readily applicable for dislocation curves near an internal free surface such as a void. By using boundary element method, which converts governing equations into also boundary integrals, the image stress due to the existence of internal surface can be computed. The merit of applying boundary element method is that only dislocated surfaces and the void surface need to be discretised, and that the surrounding infinity can be easily treated.

Compared with the classical approach of discretized dislocation dynamics (DDD) that disregards the actual shape of the dislocated surface, the proposed boundary element approach respects the arbitrariness of the dislocated surface, which can affect the displacement field caused by the dislocation [3]. Two types of geometrically necessary dislocations, namely, the prismatic dislocation loop and the shear dislocation loop have been considered in this investigation.

This study should pave the way towards an improved computational approach of modelling geometrically necessary dislocations with the presence of internal free surfaces.

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Convolution quadrature time-domain boundary element method for 2-D pure inplane anisotropic viscoelastodynamics

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Key Words: Time-domain BEM, General anisotropic elastodynamics, Convolution Quadrature Method (CQM), viscoelastodynamics, 2-D pure inplane problem

This paper presents a convolution quadrature time-domain boundary element method (CQBEM) for 2-D pure inplane anisotropic viscoelastodynamics. Since the boundary element method (BEM) is known as a suitable numerical approach for wave analysis, time-domain transient problems have been solved by many researchers using the classical time-domain BEM. However, it is known that the use of a classical time-domain BEM (TD-BEM) sometimes causes numerical instability in time-stepping procedures. In addition, the TD-BEM cannot solve wave problems with dispersion properties, such as viscoelastic and poroelastic wave problems. To overcome these difficulties, the convolution quadrature time-domain boundary element method (CQBEM) has been developed for last few decades. In the CQBEM formulation, the convolution quadrature method, first proposed by Lubich [1], is applied to the time discretization of the time-domain boundary integral equations to improve the numerical stability. The Laplace-domain fundamental solutions are utilized for the CQBEM formulation. The elastic wave scattering in viscoelastic and poroelastic solids has been analyzed by the CQBEM so far. However, no numerical examples of application of the CQBEM to the anisotropic viscoelastic wave propagation can be found as far as the authors know.

Therefore, in this study, the CQBEM for 2-D pure inplane anisotropic elastodynamics is developed by extending the previous approach for 2-D pure antiplane one [2]. In the formulation, the standard linear viscoelastic model and the fundamental solution obtained by Wang and Achenbach [3] are considered for the expression of viscoelastic and anisotropic properties, respectively. Elastic wave scattering by a cavity in anisotropic viscoelastic solids is demonstrated using the proposed CQBEM. The anisotropic and viscoelastic effects are confirmed from the numerical results to validate the proposed CQBEM.

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Development of Low Cost Solver for Incompressible Viscous Fluid Flow based on Fundamental and Particular Solutions of Differential Operator

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Key Words: *Time-Dependent Incompressible Viscous Flow, Dual Reciprocity Boundary Element Method, Fundamental and Particular Solutions*

In industrial numerical simulation of the complex and/or large scale fluid flow, the computation cost must be reduced. We develop the numerical low cost solver for the incompressible fluid flow based on the fundamental and particular solutions of the differential operator.

In the limited computational resources for the divergence of the target complexity and the size of computational fluid dynamics, the computational cost must be reduced with keeping their accuracy. The solutions for this kind problem are for example suitable modeling, the developing of computer power, the fast algorithm, or reduction of computational cell numbers.

We payed attention to the boundary element method (BEM) using fundamental solution of the diffusion operator as a potential method to solve above problem, although we know that it is effective only for the linear problems of the fluid flow, and that for the incompressible viscous flow, it needs the internal integration with the inner computational points, so BEM's potential for the reduction of computational points is not effective.

In this paper we adopt dual reciprocity boundary element method[1] as the method of transforming the internal integration to the boundary integration and boundary element formulation[2,3] which avoids using the time-dependent fundamental solution in the time integration, as the algorithm becomes simpler. By this method the transient incompressible viscous flow problems will be solved with low cost and high accuracy.

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Influence of the human body on car cabin sound field

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Key Words: *acoustic, loudspeaker, car, human body, boundary element method*

If safe autonomous driving is achieved, all passengers in a car, including the driver can participate in in-car entertainment. However, even if it is achieved, the space in a car cabin is not still ideal for listening to music because of its small space that amplifies the reflected sound from its window glasses and other road noises and vibrations. This claim has been investigated by many recent studies using computer simulations [1, 2]. The sound field within the boundaries of a car can be computer-modeled and its changes when a person enters the car. Furthermore, car loudspeakers are often located near the driver or passengers in the car. These are the focus of this study. We measured the sound field in the car when there's a person in the driver's seat. We used a traverser system and a microphone array to measure the sound pressure distribution in the car. In addition, the sound field of the analysis model was simulated using the boundary element method. The acoustic impedance of each member of the car interior was measured using the ensemble averaging method.

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Testing the use of radial basis function augmented with polynomials as basis functions in the boundary element method for heat transfer problems

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Key Words: *Radial basis function, Boundary element method, heat transfer*

The quality of the numerical solutions obtained by the Boundary Element Method (BEM) is directly affected by the type of interpolation function used for the temperature interpolation, its normal derivative and geometry along the boundary. Interpolation by radial basis function augmented with polynomials has been shown to be more accurate than Lagrange interpolation for a range of different functions.

Therefore, this paper is concerned with the application of such functions as the interpolation functions for all boundary values in the boundary element method for the numerical solution of 2d heat transfer problems. Numerical examples with different geometries and temperature distribuitions are presented and comparisons with both isogeometric and classical formulation are made to demonstrate the improved accuracy of the proposed method.

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Topology Optimization based on Level Set Method of Heat Conduction for the Heat Radiation Boundary Condition

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Key Words: Heat Radiation, Topology Optimization, Boundary Element Method, Level Set Method

Optimization problems related to heat transfers, such as heat flux maximization and thermal diffusion problems governed by Laplace's equation, are important in various engineering design applications. One of the strong approaches for solving such problems is the level-set based topology optimization method, in which the shape of the structure is updated in accordance with the distribution change of the level set function caused by updating a reaction diffusion equation of the level set function.

In the conventional studies, only Dirichlet, Neumann, and Robin type boundary conditions have been treated in the topology optimizations[1] of thermal problems, and the thermal radiation boundary condition may not have been considered so far. In the present work, we consider a topology optimization problem accompanying a thermal radiation boundary condition. The boundary element method is used for the numerical computation, because the radiation boundary condition can be written as the boundary integrals of the heat fluxes, written in the form of a double layer potential, caused by the thermal radiation, thus the BEM is advantageous in treating those boundary integrals. [2] Moreover, the BEM can be used for thermal radiation problems of an infinite space without any approximation. We consider the thermal radiation boundary condition in the augmented objective functional and take its variation when an infinitesimal cavity under the same radiation boundary condition is generated in the material. A boundary value problem accompanying only linear boundary conditions is derived as the adjoint problem, and the topological derivative expression is derived, consisting of the original radiative flux and adjoint temperature. The derived topological derivative is used as the inhomogeneous term, corresponding a source term, of a reaction-diffusion equation of the level set function. The iso-surface of distribution of the level set function is repeated by using the derived topological derivatives, which are calculated by using the BEM both for the original and adjoint boundary value problems.

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Adaptive Infill Sampling Method for Gradient-Enhanced Kriging

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Key Words: *Surrogate model, Gradient-enhanced Kriging, Adaptive infill sampling method*

Over the past few decades, surrogate models have been utilized to numerous engineering problems to increase computational efficiency, especially when optimization involves expensive computational simulations. To enhance the performances of the surrogate model, there are some representative strategies such as screening, mapping, space reduction, decomposition, auxiliary information, and hybrid methods, etc. Among the methods of using auxiliary information, gradient-enhanced Kriging (GEK), an extension of Kriging, is a good approach when cheap gradient information is available. Numerous studies show that the accuracy of GEK models is generally better than Kriging, considering the equivalent simulation time. However, unlike the Kriging, GEK modeling time is dramatically increased for high-dimensional problems, and studies are still being performed to solve this problem.
This paper proposes new adaptive infill sampling methods for GEK to efficiently build the surrogate model while maintaining accuracy. If the next infill sample is selected, the proposed method adaptively decides whether to obtain the response alone or the response and gradient together when building the surrogate modeling. The proposed methods are developed based on mean-squared error and expected improvement. Numerical examples show that the proposed methods produce better results than existing methods.

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An adaptive dimension-reduction method-based sparse polynomial chaos expansion via sparse Bayesian learning and Bayesian model averaging

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Abstract:

Polynomial chaos expansion (PCE) is widely used in the field of stochastic uncertainty quantification due to its accuracy and convergence. However, when the problems of interest are high-dimensional, PCE is usually confront with the well-known curse of dimensionality and overfitting. This study proposes an adaptive sparse learning method based on the automatic relevance determination (ARD) and the Bayesian model averaging (BMA) to solve this problem. Firstly, the sparse Bayesian learning is used to develop an analytical Bayesian compressive sensing algorithm, providing an efficient regression tool for establishing a sparse PCE model. Secondly, to improve computational accuracy and efficiency, we employ the dimension-reduction method (DRM) to reduce the size of the candidate PCE bases. Different from the common univariate and bivariate DRMs, the high-dimensional components are considered adaptively in the proposed method. Thirdly, a novel ARD method is proposed based on the concept of maximum a posterior estimation, which can prune the candidate PCE bases. The pruned PCE is regarded as an initial model, and then the BMA is used to refine the high-fidelity sparse PCE. Compared with the direct use of the noninformation prior in BMA, the initial PCE model pruned by the ARD method can improve the rationality of the prior, resulting in a better posterior estimation. For verification, two numerical examples and one engineering example are analyzed. The results show that the proposed method can achieve accurate uncertainty quantification for high-dimensional problems with limited computational budget.

Keywords: Uncertainty quantification, Polynomial chaos expansion, Dimension-reduction method, sparse Bayesian learning, Bayesian model averaging, Automatic Relevance Determination

High Dimensional Reliability Analysis using First-order Hybrid High Dimensional Model Representation and Hierarchical Kriging

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Key Words: *High Dimensional Reliability Analysis, Adaptive Kriging, Hybrid High Dimensional Model Representation, Hierarchical Kriging,*

Reliability is one of the most important factors in designing of engineering systems. Although many adaptive Kriging methods for reliability analysis have been researched, these methods are limited when they are applied to high dimensional reliability analysis problem, which is also known as the curse of dimensionality. To solve this problem, new adaptive Kriging method for high dimensional reliability analysis is proposed by adopting the concept of multi-fidelity metamodeling method.

The proposed method is composed of two adaptive Kriging methods. At the first step, adaptive Kriging method about first-order high dimensional model representation (HDMR) is conducted by adding univariate samples. With univariate samples selected by the first adaptive Kriging method, hybrid HDMR model is constructed. The proposed method is premised on the assumption that the hybrid HDMR can predict high dimensional limit-state function roughly. At the second step, hierarchical Kriging model that considers the hybrid HDMR as low-fidelity model is constructed, and adaptive Kriging method about hierarchical Kriging is conducted by adding multivariate samples. Multivariate samples are utilized not only as high-fidelity samples in hierarchical Kriging but also for estimating hybridity parameter of the hybrid HDMR, which makes full use of limited resources. The results of numerical examples show that the proposed method can evaluate accurate probability of failure more efficiently than other reliability analysis methods.

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New System Reliability Based Design Optimization Method using New Active learning function

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Key Words: *System Reliability, Reliability Based Design Optimization, Active learning function*

Uncertainties exist in complex engineering systems such as operation environment, material properties, and product dimension. Ignoring the uncertainties, the product may not satisfy the desired specification and have short life expectancy. Reliability based design optimization (RBDO) is researched to resolve these issues and applied to various mechanical systems. RBDO performs reliability analysis with a distribution of input random variables and optimizes the variables. Recently, sampling based reliability analysis methods based on Monte Carlo simulation (MCS) are widely used, and in particular, adaptive Kriging based methods have been researched. However, researches extended to optimization are insufficient, and there has not been the general system simulation cases. To resolve these issues, new system reliability based design optimization method using a new active learning function is proposed.

This research aims to solve general system reliability based design optimization (SRBDO) problems, where responses of part of constraints can be obtained by running one simulation model. The proposed method selects new sample points near the limit state functions based on new active learning function according to three types of systems, series, parallel, and combined systems. The points whose signs are certain are not selected for each constraint. System failure probability is estimated by the MCS method, and the partial derivative with respect to input random variables is also calculated to derive the SRBDO optimum. The validation results show that the proposed method effectively selects sample points near each constraint or simulation model.

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Adaptive probabilistic integration for estimation of Sobol's sensitivity indices under epistemic uncertainties

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Key Words: *Probability-box; Epistemic uncertainty; Bayesian inference; sensitivity analysis*

Owing to various sources of uncertainties existing ubiquitous in the structural parameters or external excitations, it is difficult to provide robust and reliable predictions of the behavior of engineering systems. In this regard, uncertainty quantification has been prosperously developed to properly incorporate those uncertainties in predicting system performances. This study focuses on one of the main sub-tasks of uncertainty quantification, global sensitivity analysis (GSA), for measuring how the uncertainties in model response are apportioned to model input variables, in this way to inform the relative contribution of input variables in prediction uncertainties. Among GSA techniques, variance-based sensitivity indices, which are also known as Sobol's indices, have received the greatest attention and have been widely studied by researchers from many scientific fields including computational mechanics. In classic Sobol's indices, all the input variables are assumed to follow precise probability distributions. However, due to the lack of information or limited data in many practical problems, both randomness and imprecision need to be considered in mathematic descriptions to represent aleatory and epistemic uncertainties simultaneously.

This work aims to develop an effective approach to analyze the global sensitivity of imprecisely distributed variables. Specifically, to estimate Sobol's indices of uncertain variables characterized by parametric probability-box (p-box) type. In recent years, similar problems have been investigated with a few representative research work [1][2], but they don't consider active learning strategies as well as the prediction errors in surrogate model or stochastic simulation. We propose a novel adaptive probabilistic integration procedure to explore the augmented space of both the random variables and their corresponding distribution parameters. A Gaussian process regression (GPR) model is constructed in the augmented space, then sensitivity indices of input variables are statistically inferred based on Bayesian probabilistic integration, and the marginal effects of uncertain parameters are reserved within the posterior. Utilizing the exponential squared kernel function, the formulation of posterior mean and posterior variance for Sobol's main and total indices can be analytically derived. Motivated by Ref.[3], two learning functions are designed and collaboratively work to determine the next best training point to be added into the training procedure. Once the stopping criteria are satisfied in learning both the optimization of distribution parameters and the integration of input variables, we are able to obtain accurate and robust estimations of the bounds of Sobol's indices. The ranking of the imprecise indices is further investigated based on the definition in Ref.[4]. The effectiveness of the proposed method is demonstrated with a numerical example and a Timoshenko beam.

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Computing Upper Probabilities using Global Optimization Algorithms together with Importance Sampling Techniques

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Key Words: upper probabilities, importance sampling, global optimization

Let $(X_t)_{t\in T}$ be a family of random variables $X_t : \Omega \to \mathbb{R}^d$ parametrized by t with smooth densities f_t. Then the upper probability $\bar{p} = \max_{t\in T} p(t)$ of an event D is obtained by global optimization where $p(t) = \int \chi_D(x) f_t(x)\,\mathrm{d}x$ is the probability function and χ_D the indicator function of D. In [1] we introduced the estimator $\hat{p}_{\omega,s}(t) = \frac{1}{N}\sum_{k=1}^N w_{st}(X_s(\omega_k))\cdot\chi_D(X_s(\omega_k))$ for p where $w_{st}(x) = f_t(x)/f_s^I(x)$ are the importance sampling weights for importance sampling density f_s^I corresponding to f_s. This follows from the fact that $p(t) = \int \chi_D(x) f_t(x)\,\mathrm{d}x = \int \chi_D(x)\cdot f_t(x)/f_s^I(x)\cdot f_s^I(x)\,\mathrm{d}x$. We note that in this approach all sample points $X_s(\omega_k)$, $k = 1,\ldots,N$, are based on the same fixed random numbers $\omega = \{\omega_1,\ldots,\omega_N\}$ on Ω for all $s \in T$. The special case of $s = t$ leads to the estimator $\hat{p}_\omega(t) := \hat{p}_{\omega,t}(t)$ which means classical importance sampling and using different samples for each $t \in T$. For fixed $s \in T$ the smooth function $\hat{p}_{\omega,s}$ is an approximation of $\hat{p}_\omega$ which we used in [1] to compute upper probabilities $\bar{\hat{p}}_{\omega,s}$, while here the focus is on the global optimization itself and how $\hat{p}_\omega$ and $\hat{p}_{\omega,s}$ can be used in the algorithms to compute efficiently estimates of upper probabilities.

One of the main problems for using global optimization algorithms which are not derivative-free is to compute derivatives of $\hat{p}_\omega$ because $\hat{p}_\omega$ is a step function even if the involved densities are smooth. The idea is here to use the following approximation of the partial derivatives needed for optimization: $\partial\hat{p}_\omega/\partial t_i(t) \approx (\hat{p}_{\omega,t}(t+h^{(i)}) - \hat{p}_{\omega,t}(t))/h_i^{(i)}$ with components $h_k^{(i)} = 10^{-8}\,\delta_{ik}$ of the vector $h^{(i)}$ of step sizes. We note that both estimators in the formula are based on the same sample which means that we differentiate a smooth function. A further problem is that the evaluation of χ_D may be very time consuming, e.g. finite element computations. In [1] we have seen that $\hat{p}_{\omega,s}(t)$ may be a bad approximation of $\hat{p}_\omega(t)$ for t far from s on which the sample is based and therefore not suitable to replace $\hat{p}_\omega$ by one single $\hat{p}_{\omega,s}$. Running an optimization algorithm leads to a sequence $t^{(1)}, t^{(2)}, \ldots, t^{(i)}, \ldots, t^{(j)}, \ldots$ of values. Assuming that in step i the estimator is computed in the more exact way using $\hat{p}_{\omega,t^{(i)}}(t^{(i)})$ based on the sample corresponding to $t^{(i)}$ itself, then the idea is to use an approximation $\hat{p}_{\omega,t^{(i)}}(t^{(j)})$ at $t^{(j)}$ if $\|t^{(j)} - t^{(i)}\| < \mathsf{TOL}$. This saves us N evaluations $\chi_D(X_{t^{(j)}}(\omega_k))$ because no new sample points are needed. We will apply these two methods for the algorithms in the MATLAB global optimization toolbox including examples.

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New Non-Intrusive Stochastic Finite Element Method for Geometrically Nonlinear Bending Analysis of Uncertain Laminated Composite Plates

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Stochastic finite element method (SFEM) is a kind of widely used approach for analysis of engineering structure with random properties, which can compute structural responses. For the geometrically nonlinear analysis of uncertain laminated composite plate, the existing intrusive SFEMs, such as perturbation method and spectral SFEM, have the limitations of low computational accuracy and efficiency. The versatile non-intrusive SFEM based on Monte Carlo simulation needs a great computational effort to implement a lot of expensive finite element simulations. In this paper, a novel non-intrusive SFEM is developed to achieve stochastic responses and reliabilities of laminated composite plates with geometric nonlinearity efficiently and uniformly. Firstly, the direct probability integral method (DPIM) is developed to obtain the probability density function of stochastic response of linear or nonlinear structure by solving probability density integral equation (PDIE) [1]. Secondly, the non-intrusive SFEM based on DPIM decouples the deterministic finite element analysis and PDIE to calculate the stochastic responses and reliabilities of uncertain laminated composite plates. The third-order shear deformation theory is employed to model the displacement field of laminated composite plate, and the discretization and quantification of random fields are implemented through Karhunen-Loève expansion. Finally, comparisons with the results from Monte Carlo simulation and literature show the high accuracy and efficiency of the proposed non-intrusive method. A few examples covering various features have been presented for uncertain laminated composite plates with different boundary conditions, correlation length, mean and variability of random field.

Key Words: *Laminated Composite Plates, Non-Intrusive Stochastic Finite Element Method, Direct Probability Integral Method, Random Field, Stochastic Responses and Reliabilities, Geometrically Nonlinear Bending Analysis*

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Reliability Analysis of Industrial Robot Positioning Accuracy Considering Epistemic Uncertainty

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Key Words: *Industrial robot, Reliability analysis, Evidence theory, Positioning accuracy; Uncertainty*

As one of the important equipment of intelligent manufacturing, the positioning accuracy of industrial robots has become a common concern. As a complex mechatronics product, industrial robots system have extensive aleatory uncertainties which affects its positioning accuracy reliability. In order to study the influence of epistemic uncertainty on positioning accuracy of industrial robots, this talk includes two aspects. On the one hand, an evidence-theory-based reliability analysis method through Kriging model is proposed. Kriging model is used to replace the performance function in positioning accuracy reliability analysis of industrial robots, which can achieve high efficiency and high accuracy for reliability analysis. The popular U function is used to establish the Kriging model for evidence-theory-based reliability analysis. On the other hand, a probability-evidence hybrid reliability analysis method is proposed to deal with the coexistence of aleatory uncertainty and epistemic uncertainty in industrial robots. Probability theory and evidence theory are used to describe the aleatory uncertain parameters and epistemic uncertain parameters, respectively. Random variables and evidence variables are introduced into the probability-evidence hybrid model to obtain the reliability interval of positioning accuracy of industrial robots. The reliability of positioning accuracy of industrial robots is no longer a determined value but a more objective interval. The two aspects work present a possible way to solve the problem of epistemic uncertainty of industrial robots, which can help engineers have a clear understanding of the accuracy reliability of industrial robots.

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Unified framework of computational stochastic mechanics: direct probability integral method

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Abstract: Computational stochastic mechanics involves the topics of simulation of random field or stochastic process, stochastic structural analysis, random vibration, reliability estimation and reliability-based design optimization. However, the existing methods only focus on parts of these topics, resulting in the complicated calculation and the absence of versatility. Nevertheless, the limited scope of application of approximation methods, inaccuracy and inefficiency of numerical approaches and the expensive computational cost of stochastic sampling methods restrict the development of stochastic mechanics. In this study, the novel direct probability integral method (DPIM) as a unified framework is proposed to solve the uncertainty quantification and reliability-based design optimization problems of static and dynamic structures. This method decouples the computation of probability density integration equation (PDIE) and governing equation of structures, and can achieve the probability density functions of stochastic responses and reliabilities for linear or nonlinear structural systems [1−3]. Firstly, the PDIE governing the propagation of randomness from input to output is derived based on the principle of probability conservation. The two key techniques, i.e., the partition of probability space and smoothing of Dirac delta function, are introduced to solve the PDIE. Then, the first-passage dynamic reliability based on the equivalent extreme value mapping and its sensitivity as well as reliability-based design optimization are addressed. Finally, several examples of static and dynamic structures illustrate that the DPIM is an accurate, efficient and unified methodology for uncertainty quantification and design optimization, especially for large-scale nonlinear structures under random excitation.

Key Words: *Computational stochastic mechanics, Uncertainty quantification, Static and dynamic structures, Direct probability integration method, Stochastic responses and reliabilities, Reliability-based design optimization*

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Inferential Uncertainty in Surrogate-based Inference - a Bayesian Estimate

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Key Words: uncertainty quantification, uncertainty propagation, surrogates, meta-models, emulators, Bayesian probability theory, model adequacy, surrogate uncertainty, inferential uncertainty

Uncertainty quantification is a crucial aspect of model prognosis quality assessment and often only feasible by an approximating surrogate model. One powerful aspect of Bayesian approaches [1, 2] is that it allows to treat any kind of uncertainty, model error, numerical imprecision or randomness on the same footing and with the same set of computing rules; namely as propositions [3]. Through this, we introduce and quantify the uncertainty of the surrogate itself, or its trustworthiness, as a continuous variable. This is related to what Song et al. [4] recognize as epistemic uncertainty of sensitivity index estimates. Here, this aspect is investigated for a probabilistic, generalized linear surrogate model, which includes both Polynomial Chaos Expansions and Kriging [5] as special cases, by acknowledging the uncertainty of surrogate parameter estimates. As a result, we find expressions for the evidence for, as well as the uncertainty of, the surrogate itself [6]. Then, the surrogate uncertainty is propagated to the actual Quantity of Interest (QoI). As it turns out, the surrogate's uncertainty causes an additional inferential uncertainty in the QoI that can be solely attributed to the use of an approximative surrogate. As a consequence, model predictions are easily over-confident if these inferential uncertainties are naively neglected. This fact is demonstrated with a numerical example. From this finding, a novel quality measure for surrogate models emerges naturally, without ad-hoc assumptions. This measure compares the average surrogate prediction uncertainty to its inferential uncertainty and is based on both simulation and experimental data.

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Inverting the Process-Material-Performance chain in the presence of uncertainty

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Key Words: Material design, uncertainty quantification, Inverse problem, active learning

By leveraging the power of modern high performance computing, significant advances have been made in understanding/building computational strategies for capturing nonlinear and multiscale nature of complex materials. Fewer efforts have been put into inverting the process-material-performance chain and to integrating uncertainties which are an indispensable component of materials' design. We propose a novel probabilistic framework to formulate the problem of optimization/design of material processing with respect to objectives pertaining to the performance of the systems in which material is used. A flexible, fully probabilistic formulation of such optimization problems accounts for the parameter-material property and material property-performance link and enables the identification of optimal, high-dimensional, process parameters.

We advocate the use of probabilistic data-driven surrogates for the parameter-material property and material property-performance link, that are capable of learning under Small Data, that incorporate physical constraints and are able to quantify their predictive uncertainty. Efficient tools are developed to integrate over this high-dimensional surrogates. These tools inform our novel active learning strategy, i.e. a self-supervised collection of data, which significantly improves accuracy while requiring small amounts of training data. We demonstrate the efficacy of the framework for different systems in which concrete is used and report on its performance.

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Investigation of complex-valued correlation models for model updating with spatially distributed data

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Key Words: *Uncertainty quantification, Bayesian updating, Structural dynamics, Frequency response function, Correlation models.*

Bayesian system identification determines the parameters of models from measurements of the system response. The underlying inverse problem is formulated in a probabilistic setting, and Bayes' rule is applied to update a prior conjecture on the parameters with the data. We apply the Bayesian framework to identify the parameters of structural systems using frequency domain measurement data. The likelihood function expressing the measurement information is formulated in terms of the misfit of the data and the model frequency response function. Often, it is assumed that the model misfit between different observations is uncorrelated. It can be shown, however, that this assumption does not hold in general and that neglecting the correlation between observations leads to poor estimates of the posterior distributions [1]. In this study, we focus on the investigation of correlation models that describe the autocorrelation of the model error in the spatial and frequency domain. Previous approaches have used standard correlation models, such as the exponential model, to account for the correlation between different points [1,2]. In [2], we interpret the model error as a complex random variable. In this contribution, we propose a complex-valued correlation function to describe the model error correlation. Furthermore, we investigate models that include a sinusoidal pattern to take into account the periodicity in the system response. The proposed models are successfully applied to identify the stiffness and damping parameters of a finite element model of a plate structure. We evaluate the performance of the different correlation models by comparing their evidence.

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Real-time structural health monitoring of aeronautical structures: A data-driven modeling approach for optimized sensors placement, detection and localization of damage

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Key Words: *structural health monitoring, aeronautical structures, data-driven modeling, model order reduction, sensors.*

Real-time structural health monitoring represents a valuable service for airlines and the aeronautical industry in general. Indeed, planned preventive maintenance based on accurate forecasting would increase the safety of operations and reduce their costs. Structural health monitoring consists in the automated implementation of a strategy to determine the health status of a structure at regular intervals.

The present work investigates a methodology of real-time structural health monitoring of an aircraft engine fan blade equipped with a minimum set of sensors placed in an optimized way to detect and locate degradations. Recent technological advancements in sensors have led to a significant interest in data-driven modeling techniques for structural health monitoring [1]. Following this trend, an undamaged data-driven model that uses proper orthogonal decomposition to compress a database comprising static and dynamic displacements was developed. The proposed method relies on a sample of fluid structure simulations and provides good approximate solutions with a reduced calculation time by exploiting a pre-constructed reduced basis.

This reduced basis can also be used to define an optimized sensors placement on the structure. Indeed, the obtained data must allow the accurate reconstruction of the displacement field. However, usual methodologies used for optimal sensors placement, such as discrete empirical interpolation and QR-pivoting, are limited because the number of sensors is correlated with the truncation of the reduced basis. The present work proposes a new methodology for sparse sampling that allows a full signal to be reconstructed from a small subset of measurements. This subset is constructed assuming that the number of sensors is greater than the size of the reduced basis. The sensors can detect every damage and are placed in a non-redundant way to avoid aggregation problems on the physical structure [2]. The methodology provides a robust and instantaneous full-state reconstruction of the displacements and therefore allows a reliable detection and accurate localization of the onset of an anomaly on the structure.

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Tunnel Lining Deformation Prediction Using Limited Measurements And Gappy Proper Orthogonal Decomposition

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Key Words: *proper orthogonal decomposition, tunnel lining, missing data, numerical simulation, mechanized tunnelling, real-time simulation*

Mechanized tunnelling is a flexible and efficient technology for the construction of underground infrastructure. As the main structure of a tunnel, tunnel linings are designed to permanently fulfil basic structural, serviceability and durability requirements throughout the lifetime of a tunnel. Therefore, it is important to correctly assess the response of the tunnel lining with respect to the loads from the ground and from the tunnelling process to which lining structures are subjected in order to ensure the structural reliability [1]. In general, tunnel lining deformations are monitored using only a limited number of sensors installed at specific locations around the tunnel.

In this work, a simulation-based approach is presented, which allows predicting the complete tunnel lining deformation using the limited sensors information in combination with the Gappy Proper Orthogonal Decomposition method [2]. In this approach, a numerical simulation model is employed to simulate the complete tunnel lining behaviour under different possible loading scenarios. The real sensor measurements at limited locations are then utilized together with the simulation data in the context of a reconstruction problem to predict the behaviours at other locations around the tunnel. This allows to get a real-time response of the tunnel lining deformation field, which can be used to assess the current structural reliability. Additionally, the approach can also provide suggestions of locations around the tunnel where the sensors should be installed in order to maximize the prediction accuracy of the presented approach.

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Accelerating a Nonparametric Probabilistic Method for Physics-Based Data-Driven Modeling and Uncertainty Quantification

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Key Words: *data-driven modeling, stochastic optimization, uncertainty quantification*

The nonparametric probabilistic method (NPM) presented in [1] for modeling and quantifying uncertainty is a multi-faceted, data-enhanced, computational modeling method. Because it is grounded in projection-based model order reduction, it is data-driven – even in the absence of experimental data – and computationally tractable. Essentially, NPM is a physics-based, machine learning method for extracting from data fundamental information and/or knowledge that are not captured by a deterministic, high-dimensional computational model (HDM) of dimension N, and infusing them into a counterpart stochastic, projection-based reduced-order model (PROM). Starting from a deterministic HDM, NPM constructs in three steps a counterpart stochastic, hyperreduced PROM (SHPROM). First, it builds a deterministic PROM of dimension $n \ll N$ and hyperreduces it. Next, it substitutes the deterministic Reduced-Order Basis (ROB) underlying the PROM with a stochastic counterpart (SROB) that it constructs on a subset of a compact Stiefel manifold, using a number of hyperparameters that grows as of $O(n^2)$. Finally, it identifies the hyperparameters by formulating a statistical inverse problem such that the mean value and statistical fluctuations of some quantities of interest predicted using the resulting SHPROM match target values obtained from data; and solving the corresponding optimization problem.

While the potential of NPM for quantifying model-form uncertainties has been successfully demonstrated for a number of applications [2], its practicality is contingent upon the computational tractability of the solution of the optimization problem underlying the identification of its hyperparameters. This problem is non-convex, stochastic, and therefore computationally intensive. So far, it has been solved using gradient-based methods where the sensitivities of the objective function with respect to the hyperparameters are computed by finite differencing, which has raised robustness and performance issues. For highly nonlinear HDMs where the SHPROM has typically a dimension $n \geq 20$, these issues are exacerbated by the larger size of the stochastic optimization problem. Here, they are addressed by a two-pronged approach. First, NPM's inverse statistical problem – and therefore its number of hyperparameters – is reduced from $O(n^2)$ to $O(n)$ by developing a network of autoencoders that provide a nonlinear approximation of the dependence of the randomized reduced-order basis on its hyperparameters. Second, the sensitivities of the objective function of the optimization problem with respect to the hyperparameters are computed analytically, by tracking the complex web of operations underlying the construction of the stochastic objective function. The net result is an implementation of NPM whose robustness and performance are dramatically improved. These improvements and the potential of the enhanced NPM for the physics-based, data-driven modeling of solid mechanics / structural dynamics problems and the reduction of their model-form uncertainty is demonstrated on an application pertaining to a jet engine nozzle problem.

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Impact Problems on Dyadic Tensor-Valued Random Fields

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Key Words: Impact Problems, Dyadic Random Field, Wave Propagation, Response Amplitude

We report a study of impact problems on random fields. First, an impact model is formulated as a boundary value problem for a stochastic partial differential equation, where the randomness is incorporated into the differential operator with the help of two homogeneous and isotropic random fields, one of each is scalar-valued and describes the mass density, and another one is rank 2 symmetric tensor-valued and describes the stiffness. See [1] for detailed description of the above approach.

Our study is an extension of the previous studies [2, 3]. We suppose that the stiffness random field governing the impact dynamics is represented as the sum of the deterministic mean value and a positive-definite dyadic product of two vector-valued Gaussian random fields. For the latter fields, we suppose that their spectral densities belong to a prescribed parametric class. Using the Monte Carlo simulation approach, we study the mean response amplitude and the sensitivity of wave propagation for a wide range of parameters that describe the fractal dimension and Hurst parameter of the governing fields.

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Information-Theoretic Stochastic Models for Uncertainty Quantification in Computational Plasticity

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Key Words: Anisotropic Plasticity, Hill Coefficients, Information Theory, Stochastic Modeling, Uncertainty Quantification

While uncertainty propagation through plasticity models has been studied quite extensively, either by means of Monte Carlo simulations or by using polynomial chaos expansions, contributions focusing on the proper modeling of stochastic input parameters in computational plasticity remain very scarce. In this work, we address the construction of information theoretic stochastic models, and focus on the case of anisotropic Hill plasticity. A formulation involving a low-dimensional parameterization is first laid down. We subsequently apply the framework to model variations observed in physical experiments on materials processed by additive manufacturing. Uncertainty propagation is finally conducted to gain insight about the impact of material variability on the structural response of complex structures.

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A Painless Automatic *hp*-Adaptive Coarsening Strategy For Non-SPD Problems: A Goal-Oriented Approach

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Key Words: *hp*-Adaptivity, Goal-Oriented Adaptivity, Unrefinements, Finite Elements

In the context of *hp*-adaptivity, Darrigrand et al. [1] introduced a novel automatic mesh-refinement strategy based on a multi-level hierarchical data structure proposed by Zander et al. [2]. Darrigrand et al. [1] algorithm marks the basis functions with the lowest contributions to the energy of the solution. It removes them to achieve an automatic *hp*-adaptive strategy built upon an unrefinement process that optimizes the existing computational resources. However, the global energy of the problem may be a quantity of limited relevance. Thus, many engineering applications require the approximation of a specific Quantity of Interest (QoI). Mesh adaptive algorithms intended to approximate a specific QoI are known as Goal-Oriented adaptive algorithms (see, e.g., [3-4]). They look for an accurate approximation of the QoI using an error estimator to guide refinements based on the solution of the dual problem. In this presentation, we extend the previous work [1] to goal-oriented symmetric positive definite (SPD) and non-SPD problems, re-defining the contribution to the energy to take into account both the direct and the adjoint problem. We test and analyze our algorithm on two-dimensional (2D) Poisson and Helmholtz problems, and we describe the main features and limitations of the proposed method. In particular, our algorithm is robust and straightforward to implement; therefore, it can be used for industrial applications.

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A posteriori analysis with error-dominated oscillation for higher order methods

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Key Words: Adaptive finite element methods, a posteriori error estimates, higher order methods

In a posteriori error analysis, the relationship between error and estimator is usually spoiled by so-called oscillation terms, which cannot be bounded by the error. In order to remedy, [1] devised a new approach for the standard linear finite element method where the oscillation has the following two properties. First, it is dominated by the error, irrespective of mesh fineness and the regularity of data and the exact solution. Second, it captures in terms of data the part of the residual that, in general, cannot be quantified with finite information. The new twist in the approach is a locally stable projection onto discretized residuals. In the case of the Poisson problem, the approach leads to an improved standard residual estimator and allows tackling problems with sources in H^{-1}.

We shall present a generalization of this approach to higher order methods.

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Adaptive Concurrent Multiscale Modelling Using Hybridized Discretizations, Error Estimation and Machine Learning

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Key Words: *Multiscale modelling, adaptive modelling, error estimation, hybridized discretizations, machine learning*

Multiphysics systems are often strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a large range of length- and time-scales. Performing direct numerical simulation of such systems that resolves all the relevant length- and time-scales is often prohibitive, even on the modern leadership-class computing platforms. Nevertheless, these fine-scale variations often impact the behaviour of the system on a much larger scale in non-negligible ways. Thus, one often seeks to model or approximate the subgrid scale phenomena to accurately and efficiently capturing their impact on the coarse scale solution. Multiscale formulations based on non-overlapping domain decomposition methods have the additional benefit of allowing different physical models and numerical discretizations in different regions. However, determining the optimal subgrid model within a coarse scale region that effectively balances accuracy and computational expense can be challenging for transient nonlinear multiphysics applications.

In this presentation, we describe our theoretical and computational frameworks that are based on a generalization of hybridized discretizations and are designed to exploit heterogeneous computational architectures to enable concurrent multiscale modelling on a range of transient nonlinear multiphysics applications. We will also describe our utilization of dynamic adaptive subgrid modelling and how we are utilizing a posteriori error estimation procedures and supervised machine learning strategies to determine the appropriate subgrid model for an element in the coarse scale partition. We will provide demonstrations on applications motivated by subsurface flow and mechanics in porous media and additive manufacturing.

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Adaptive Stochastic Collocation Methods for Uncertain Unsteady Gas Transport in Networks

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Key Words: *uncertainty quantification, adaptivity, stochastic collocation, gas transport in networks, model hierarchy, balance laws, Euler equations at junctions*

In this talk, we will present recent results for the quantification of uncertainties that arise from intra-day oscillations in the demand for natural gas transported through large-scale networks [2]. The short-term transient dynamics of the gas flow is modelled by a hierarchy of hyperbolic systems of balance laws based on the isentropic Euler equations. We extend a novel adaptive strategy for solving elliptic PDEs with random data, recently proposed and analyzed in [1] to uncertain gas transport problems. Sample-dependent adaptive meshes and a model refinement in the physical space are combined with adaptive anisotropic sparse Smolyak grids in the stochastic space. A single-level approach, which balances the discretization errors of the physical and stochastic approximations, and a multi-level approach, which additionally minimizes the computational costs, are considered. Two examples taken from a public gas library demonstrate the reliability of the error control of expectations calculated from random quantities of interest, and the further use of stochastic interpolants to, e.g., approximate probability density functions of minimum and maximum pressure values at the exits of the network.

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Anisotropic adaptive finite elements for aluminium electrolysis

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Key Words: Aluminium electrolysis cells, anisotropic adaptive finite elements, anisotropic error indicator, nonlinear p-Laplace problem

Anisotropic, adaptive finite elements have shown to be very efficient for solving pde's with boundary or internal layers. The application to fluid flow in aluminium electrolysis cells will be presented, where two immiscible, incompressible and turbulent fluids are involved. Using the anisotropic error indicator presented in [1] for Stokes' problem, anisotropic adapted meshes will be used to produce accurate results with far less vertices than uniform meshes.

The error indicator will be justified on the simplified nonlinear problem (some kind of p-Laplace problem):

$$-\text{div}\,((\mu+|\nabla u|)\nabla u) = f,$$

where μ corresponds to the laminar (constant) viscosity and $|\nabla u|$ to a turbulent (Smagorinsky) viscosity. Numerical experiments will show that the use of quasi-norms as in [2] is needed to obtain effectivity indices close to one.

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Data-based Model Updating, Selection, and Enrichment using the Modified Constitutive Relation Error Concept

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Key Words: Inverse analysis, Hierarchical model selection, Data-based enrichment

In the context of computational engineering, physical systems are classically represented by a mathematical model which can be picked in a hierarchical list of possible models, with increasing complexity, and which is then numerically processed to obtain a virtual twin. In such a framework, a critical error source comes from imperfect modeling. Therefore, for safe decision-making, there is a need for certification of the predicted outputs, with consistency between physical reality and numerical models; this is the matter of model parameter updating, but also model enrichment in order to correct model bias from data-based information (hybrid approach). On the other hand, there is a need for effectivity, in order to perform fast data assimilation and control as required in Dynamic Data Driven Application Systems (DDDAS) in which a continuous exchange between simulations and experimental measurements is implemented. The goal is thus to compute right at the right cost, with smart management of computing resources depending on the objective and complexity of the observed physical phenomena. This resorts to model adaptivity and suitable selection of a reference mathematical model in view of experimental data.
The talk addresses these various topics by using the Constitutive Relation Error concept. In its modified version [1, 2], it is a powerful, relevant, and robust tool to perform suitable modeling and simulation with respect to experimental information. During the presentation, the philosophy and performance of this tool will be shown on several recent mechanical engineering applications related to (sequential) model parameter updating with noisy data (e.g. [3]), but also data-based model selection and correction with regards to rich data coming from full-field measurements or distributed optic fiber sensing.

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Goal-oriented adaptive MLMC method for elliptic random PDEs

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Key Words: Goal-oriented adaptivity, MLMC, Matérn random fields, ellptic random PDE

Multilevel Monte Carlo methods (MLMC) can dramatically reduce the computational cost of Monte Carlo simulations where each sample is computed using a discretization based numerical method, for example, when computing the expected value of a quantity of interest (QoI) depending on the solution to a partial differential equation with stochastic data.

Goal-oriented adaptive finite element refines the mesh based on the error contribution to the QoI. The method is effective, for instance, when the geometry presents a singularity, such as a non-convex domain.

The purpose of this work is to combine MLMC and adaptive finite element solvers, to efficiently solve a boundary-value problem of an elliptic partial differential equation with random coefficients on a non-convex domain. The QoI is a linear functional of the PDE solution, and the coefficient field is efficiently sampled from a regular coefficient random field. The adaptive refinement algorithm is based on [1]. This work can also be seen as an extension of [2].

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Mesh Adaptivity using Optimization Methods

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Key Words: A posteriori Error Estimation, Optimal Transport, Minimization Problems with Constraints

The talk will deal with the development and analysis of optimal approaches for mesh adaptation for the discretization of classical boundary-value problems. One can mathematically show that some greedy adaptive methods provide optimal rates of convergence with respect to the energy norm or some quantity of interest for simple problems such as those given in terms of symmetric positive-definite boundary-value problems [1, 2, 3]. Performance of the methods for general problems is far less clear. The objective of the talk will be to reformulate mesh adaptivity in terms of minimization problems with constraints, based either on classical optimization theories [4, 5] or on concepts from optimal transport [6]. The performance of the different formulations will be compared on classical model problems.

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On Error Control and Adaptive Reduced Basis Enrichment for Two-Scale Poroelasticity

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Key Words: *Porous media, Computational Homogenizaition, Reduced Order Modeling, Error Control*

The problem of determining the mechanical response of heterogeneous fluid-saturated porous rock using computational homogenization is considered. One standard approach is the so-called "finite element squared" (FE^2) procedure, where a new boundary value problem for the coupled porous media problem is defined on a Representative Volume Element (RVE) in each macroscopic quadrature point. In the case of non-linear or transient effects, the effective response must be computed on the fly, making the strategy computationally intractable in practice for detailed RVE-structures. It is therefore of interest to reduce the cost of solving the individual RVE problems by introducing a reduced basis, here denoted Numerical Model Reduction (NMR).

Computational homogenization using NMR was presented by Jänicke et al. [1], considering Proper Orthogonal Decomposition (POD), and extended by Ekre et al. [2] where an a posteriori error estimator was presented. In addition to POD, Spectral Decomposition (SD) was also used for basis generation in the latter work. It was shown that the POD basis outperforms the SD basis in terms of accuracy, but the SD basis behaves better in that it did not overestimate the error as much.

In this contribution, we complete the computational strategy by presenting a novel procedure for adaptively enriching the NMR-basis with either POD- or SD-basis functions using a refinement indicator derived from the error estimator. Previous work is also extended by considering non-linear modelling in terms of deformation-dependant permeability. The generation of POD-basis is unaffected by the non-linearity and the generation of spectral modes can still be carried out based on a linearization. However, the accuracy of the reduced approximation typically reduces with the amplitude of the non-linearity. The previously developed error estimator is linearized in a manner that it presents guaranteed bounds on the error in the limit of infinitesimal loading.

We study a few numerical examples of 3D RVE-structures, where we seek the effective response during prescribed loading of varying amplitude. The robustness and accuracy of the linearized error estimate and the efficiency of the adaptive basis enrichment procedure are investigated.

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Optimality of Adaptive Time-Stepping

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Key Words: adaptive mesh refinement, optimality, error estimation, non-stationary problems

In the recent work [1], we prove new optimality results for adaptive mesh refinement algorithms for non-symmetric, indefinite, and time-dependent problems by proposing a generalization of quasi-orthogonality which follows directly from the inf-sup stability of the underlying problem. This completely removes a central technical difficulty in modern proofs of optimal convergence of adaptive mesh refinement algorithms and leads to simple optimality proofs for the Taylor-Hood discretization of the stationary Stokes problem, a finite-element/boundary-element discretization of an unbounded transmission problem, and an adaptive time-stepping scheme for parabolic equations. The main technical tool are new stability bounds for the LU-factorization of matrices together with a recently established connection between quasi-orthogonality and matrix factorization.

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Polynomial-degree-robust a posteriori error estimation for the curl–curl problem

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Key Words: equilibrated flux reconstruction, Maxwell's equations, Sobolev space $\boldsymbol{H}(\mathrm{curl})$, Sobolev space $\boldsymbol{H}(\mathrm{div})$, p-robustness, a posteriori error estimate, divergence-free decomposition

A posteriori error estimates by flux equilibration are nowadays well established for many model problems. This is, however, not the case for the curl–curl problem, as a simplification of Maxwell's equations. In this contribution, we describe two novel estimates for its Nédélec finite element discretization.

In the first case, we avoid the use of the Prager–Synge equality. We devise a "broken patchwise equilibration", relying on small patches of tetrahedra around the edges of the mesh. Mathematically, this is related to the localization of the residual with test functions in $\boldsymbol{H}_0(\mathrm{curl})$. The resulting estimators are reliable, locally efficient, and polynomial-degree-robust, but contain some (computable) constants.

In the second case, we design a full equilibration in that we construct a $\boldsymbol{H}(\mathrm{curl})$-conforming Nédélec piecewise polynomial with a prescribed curl. Our procedure relies on larger patches of tetrahedra around vertices and is mathematically related to the localization of the residual with test functions in $\boldsymbol{H}(\mathrm{curl})$ and to a divergence-free decomposition of a given divergence-free $\boldsymbol{H}(\mathrm{div})$-conforming Raviart–Thomas piecewise polynomial. The resulting estimators are here reliable, locally efficient, polynomial-degree-robust, and constant-free, since obtained via the Prager–Synge equality.

Stable extensions of piecewise polynomial data prescribed in a patch of tetrahedra sharing an edge/vertex are a central theoretical tool. Numerical results illustrate the theoretical developments. This is a joint work with Alexandre Ern (first case, [1]) and with Théophile Chaumont-Frelet (both cases, [1, 2]).

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Revisiting techniques employed in error estimation for their use in 2-level structural topology optimization with the Cartesian grid FEM.

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Key Words: *Topology optimization, Superconvergent Patch Recovery, statically admissible stress field, equilibrated tractions*

In 2-level topology optimization (TO), an initial TO iteration run on a coarse mesh (the macro-level) is followed by a TO iteration run on a fine mesh (meso-level) at each of the cells defined by the elements of the macro-level. In structural applications, the boundary tractions applied on each cell of the meso-level are evaluated from the FE stress field of the macro-level. Geometrical continuity between adjacent cells is required in structural applications for a proper load transference between cells. This geometrical continuity cannot be obtained if different traction distributions are applied on the shared faces of adjacent cells. Hence, this geometrical continuity cannot be achieved considering the FE stress field, obtained at the macro-level, since tractions acting on conforming element faces that equilibrate with an internal stress field do not usually maintain the element in equilibrium, and neither are they codiffusive with adjacent elements. Thus, for 2-level TO, we need to postprocess the FE stress field of the macro level to obtain a stress field that provides both, the traction continuity between adjacent cells and the equilibrated tractions at each cell. Hence, we would need a statically admissible stress field.

In this work, and in the framework of the Cartesian grid FEM (cgFEM) [1], we revisit the use of two techniques aiming at evaluating statically admissible stress fields, previously developed in the traditional context of discretization error bounding/estimation. On the one hand, we will consider the process based on the use of graphs showing the interactions between neighbour elements and Maxwell force diagrams [2] used by Ladevèze in the Constitutive Relation Error method. On the other hand, from the context of the Recovery-based error estimators developed by Zienkiewicz, we consider an extension of the Superconvergent Patch Recovery (SPR) technique, the SPR-C technique [1], that uses constrain equations to ensure the satisfaction of the internal and boundary equilibrium equations at patch level. This work analyses the behaviour of these two techniques in 2-level TO.

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TOWARDS AUTOMATED COMPUTATION WITH UNCERTAINTY ESTIMATION FOR INDUSTRIAL SIMULATION OF SHIP FLOW

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Key Words: Mesh adaptation, Automatic simulation, Mesh convergence, Ship resistance

Mesh generation is a bottleneck for the current industrial use of CFD, due to its dependence on expert user knowledge and its unpredictable cost, since iterative modification of the meshes may be needed to correctly resolve flow features. Adaptive mesh refinement is a natural solution to these problems. However, mesh adaptation is only acceptable in an industrial context if it can be performed automatically, with little or no user intervention, and if it is robust enough to produce reliable solutions for a large range of test cases.

This paper studies the use of adaptive refinement for the industrial simulation of free-surface water flows. We ensure the reliability of the simulation results by two means. First, the computational setup is automated; physics-based arguments are used to derive guidelines to automatically set the simulation parameters correctly for each simulation, independent of the flow conditions and the geometry [2]. With these parameters, adaptive meshing produces grids that are suitable for capturing each flow.

Furthermore, the metric-based refinement criteria that we use make it easy to produce series of coarse to fine meshes, which can be combined with classical numerical uncertainty estimation procedures [1]. It is shown that the grid convergence obtained is remarkably smooth for unstructured meshes, which implies that the estimated uncertainty bounds are sharp and accurate.

The procedure is demonstrated for the resistance evaluation of ships. A first test case is used to fine-tune the simulation guidelines, which are then applied unchanged to three other ships, ranging from a destroyer to a supertanker. In all cases, the simulation results are good, which proves the generality of the approach. Thus, the mesh adaptation and uncertainty estimation procedure appears powerful and reliable enough for routine use in industry.

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Manufactured Solutions for the Method-of-Moments Implementation of the Electric-Field Integral Equation

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Key Words: Method of Moments, Electric-Field Integral Equation, Code Verification, Manufactured Solutions

Though the method-of-moments implementation of the electric-field integral equation plays an important role in computational electromagnetics, it provides many code-verification challenges due to the different sources of numerical error. In this talk, we provide an approach through which we can apply the method of manufactured solutions to isolate and verify the solution-discretization error. We accomplish this by manufacturing both the surface current and the Green's function. Because the arising equations are poorly conditioned, we reformulate them as a set of constraints for an optimization problem that selects the solution closest to the manufactured solution. We demonstrate the effectiveness of this approach for cases with and without coding errors.

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Considering epistemic uncertainty in optical marker based joint angle calculation during human gait

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Key Words: Epistemic uncertainty, Uncertainty modelling, Uncertainty propagation, Soft tissue artifacts, Human gait, Joint angle calculation

Joint angles during human gait are commonly computed from data measured via optical marker based motion capture [1]. For this, markers are placed on the human body and their position is tracked with cameras. Based on the measured positions paired with the correlation of the placement of markers relative to the person's physiology, the joint angles and segment positions can be calculated and evaluated. This process has multiple sources for uncertainty. The measurement of the marker positions as well as their position on the body is affected by uncertainty. Furthermore, due to the relative motion between bones and skin, soft tissue artefacts (STAs) further increase the uncertainty.

In this work, we examine the different causes for uncertainty in the measurement and calculations and propagate it forward, using an epistemic (fuzzy) uncertainty model and α-level optimisation [2, 3]. For each marker, we assume that it's true position is within a sphere around the measured position, whose radius is modelled by a convex fuzzy number. This means the radius can vary within an interval and each value within this interval is assigned a membership value, based on the membership function. The resulting envelopes of the joint angles are then calculated with α-level optimisation, allowing for efficient propagation of the uncertain marker position and to calculate the uncertain joint angles. This enables the analysis of joint angle values with respect to the uncertain input parameter. Different joint angles during gait are examined. The results are discussed with respect to uncertainty modelling and its propagation through the joint angle calculation.

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Data-Driven Computational Homogenization of Polymorphic Uncertain Material Properties

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Key Words: Data-Driven Mechanics, Numerical Homogenization, Polymorphic Uncertainty, Data Science, Nearest Neighbor search

The macroscopic behavior of composite materials (e.g. steel or carbon reinforced concrete) is strongly dependent on the mesoscopic heterogeneities. Based on numerical homogenization methods, which are premised on the concept of scale separation, the mechanical behavior of the mesoscale is considered within the structural analysis of the homogeneous macroscopic replacement continuum. The heterogeneous mesoscopic material behavior is characterized by a representative volume element (RVE) with uncertain properties. The realistic modelling of structures requires the consideration of aleatoric and epistemic uncertainty. Generalized polymorphic uncertainty models (p-box, fuzzy probability based randomness with bunch parameter description) are utilized in order to take variability, imprecision, inaccuracy and incompleteness of material data into account. The concept of data-driven computational mechanics [1] enables material model free finite element analyses of solids directly based on stress-strain data sets. The key idea is to assign a state which fulfills equilibrium and compatibility constraints and leads to a minimum of the penalized objective function to every integration point. Thus, the data-driven computation scheme incorporates methods for solving nearest neighbor searches (e.g. k-d tree, ball tree).

A data base characterizing the macroscopic material behavior is derived by solving the boundary value problem of the displacement-driven RVE for varying deterministic boundary conditions and quantifying the polymorphic uncertainty of the corresponding stresses resulting from the uncertain mesoscopic material parameters. A computationally efficient approach for the consideration of data sets containing uncertain stress-strain states within data-driven computation based on information reduction measurements and efficient nearest neighbor search algorithms will be developed. Due to the generalization, the approach is applicable to various aleatoric, epistemic and polymorphic uncertainty models. In addition, different phase space sampling strategies are adapted to the data-driven solver and compared. The workflow and characteristics of the developed methods are demonstrated by structural examples with polymorphic uncertain mesoscopic material properties quantified by p-boxes.

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Homogenization and dimension reduction of elastic rods with randomly perturbed geometry

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Key Words: Additive Manufacturing, Uncertainty Quantification, Homogenization, Surrogate Models

For a period of time now, additive manufacturing has been a widespread method in a huge variety of engineering applications. Thereby its nearly limitless design freedom has enabled the practice of trial and error approaches in many fields like bio-engineering or civil-engineering, see for instance [1]. However one aspect that has only recently been investigated is the error introduced in the designs due to the manufacturing process. In this context small-scale variations of the material properties (e.g., density fluctuations) and mesoscopic geometric deviations can often be considered as main sources of uncertainty. Indeed the variability in certain mechanical properties of additively manufactured slender elastic rods is significant, see for instance [2]. Quantifying the effect of such deviations on different mechanical properties of slender elastic rods numerical techniques based on finite element methods for 3D solids combined with Monte-Carlo methods are very well known. Unfortunately such methods usually exhibit extremely high computational cost and often turn out to be impractical in the ordinary usage. This is a special limiting factor as besides uncertainties of aleatoric type (following a well-characterized probability distribution) some errors introduced in the printing process are more difficult to quantify and thus fall in the epistemic category where for example only bounds on probabilities can be established (e.g., due to difficulties in imaging the printed objects using computer tomography). In order to quantify the impact of random deviations in a more efficient way simplified and at the same time accurate surrogate models were derived in the present work using dimension reduction and recently developed mathematical methods in quantitative homogenization leading to a marked reduction in computational effort.

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Multifidelity Moving Particles via Multiplicative Information Fusion

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Key Words: Moving Particles Method, Information Fusion, Multifidelity, Multivariate Expectation Maximization

In structural reliability analysis the Monte Carlo method (MC) is often used to compute the Probability of Failure (PoF) since analytical solutions are not available. More often than not, the model to be evaluated has a demanding computational cost which makes MC infeasible, due to the high number of samples needed to describe the rare event. With regard to polymorphic uncertainties, the demand increases even further since the PoF's upper and lower bound are computed in a double loop at additional cost [1].

The moving particles method offers significant improvements over plain MC and the number of evaluations is reduced drastically. Here, a small number of samples (particles) is created by MC and then moved into the failure domain by applying Markov Chain Monte Carlo. This leads to a Poisson process whose parameter is linked to the PoF. [2]
To further increase the efficiency, a multilevel version has been introduced recently which combines multiple models of different fidelity via additive information fusion [3].

In a first step to efficent sampling methods for polymorphic untertainties, a new approach is proposed which focuses on aleatoric uncertainties only and uses multiplicative information fusion. Therefore, Expectation Maximization is applied to estimate the Poisson parameter of the high fidelity model. This is achieved in two ways: On the one hand the parameters of a multivariate Poisson distribution [4] are estimated using all models at once, adapted for decreasing samples per fidelity level. On the other hand the models are combined pairwise leading to a step by step solution with a bivariate Poisson distribution estimation in each step. Both versions are tested on an example and afterwards compared with regard to relative error and computational time.

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Polymorphic Uncertain Dependency Structures in Multivariate Fuzzy Probability-based Random Variables with Fuzzy Probability-based Copula

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Key Words: Uncertainty Quantification, Polymorphic Uncertainty, Dependency Structure, Copula

Copulas are commonly applied to characterize and incorporate dependency structures of multivariate random variables in stochastic uncertainty quantification. For the modeling of copulas, e.g. based on measurement data of the multivariate random variable, copula-parameter estimation methods are required.

In the context of polymorphic uncertainty, on the one hand, aleatoric uncertainty characteristics, commonly based on stochastic uncertainty models and, on the other hand, epistemic uncertainty characteristics, e.g. based on fuzzy or interval uncertainty models, are distinguished and both uncertainty characteristics are considered in combined uncertainty models. Multivariate fuzzy probability-based random variables are investigated as polymorphic uncertainty model, combining the uncertainty characteristics by fuzzy-parametrization of probability functions and, according to [2], fuzzy-parametrized dependency structures.

Two novel approaches are presented to model polymorphic uncertainties in dependency structures based on copulas. The approaches are extending present methods of copula-parameter estimation and both are resulting in fuzzy-parametrized copula models, accordingly denoted as fuzzy probability-based copulas.

In the first approach, dependency structures in multivariate random variables are investigated. In [1], methods for interval-valued copula-parameter estimation are proposed, which are characterized by confidence interval estimators. Based on this, an estimator for fuzzy-parameterized copulas is developed. In the second approach, fuzzy-parametrized marginal probability functions are investigated. An additional fuzzy analysis is introduced to estimate the fuzzy copula-parameters. The developed method enables the estimation of copulas as dependency structure of the polymorphic uncertain multivariate variable.

Novel data based estimator methods are developed for both approaches. Therefore, the applicability of the approaches is shown by numerical examples, where uncertainty quantification is performed for a structural problem of a timber construction, based on measurement data of sensitive system parameters.

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Reliability-Based Design Optimization under Polymorphic Uncertainties: Application to Locally Laser-Hardened Car Components

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Key Words: reliability-based design optimization, optimal uncertainty quantification, polymorphic uncertainties, local laser-hardening

To ensure the safety of engineering structures under the influence of polymorphic uncertainties, optimal designs can be obtained from reliability-based design optimizations (RBDO). Therein, the computation of the mathematically sharpest (upper) bound on the probability of failure (PoF) is a crucial task, since the computed bound on the PoF is compared to a specified threshold to evaluate the safety of a design candidate. In this context, no uncertified assumptions in terms of probability density functions on the uncertain input quantities should be made to avoid faulty results from the optimization. Under this premise, the extended Optimal Uncertainty Quantification (OUQ) is a suitable framework for the uncertainty quantification, cf. [3] for the original approach and [2] for its extension to polymorphic uncertainties. The key feature is the ability to incorporate information on moments of epistemic quantities without an assumption on the type of an underlying probability density function while still enabling the inclusion of probability densities for description of aleatory uncertainties. Thereby, uncertified assumptions on the data are avoided and the safety of the design is maintained. In this contribution, the integration of the extended OUQ framework in an RBDO-context is presented. For that matter, the production process and crash behavior of a car front bumper under the influence of polymorphic uncertainties including uncertain sheet metal properties resulting from microstructure variation [1] are numerically evaluated. Therein, the arrangement of locally laser-hardened zones in the sheet metal is optimized in order to maximize the dissipated energy of the front bumper in a simple crash scenario. Since individual computations of each design candidate in terms of finite elements are costly, a surrogate model is constructed, which is then used in the RBDO itself for efficiency reasons.

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A trial for validating the model of reinforced concrete beams with emphasis on uncertainty quantification

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Key Words: *ASME V&V 10, uncertainty quantification, smeared crack model, finite element method, reinforced concrete*

In the design of reinforced concrete (RC) structures and the development of construction methods, the current mainstream is the use of experiments. However, this method requires a lot of preparation and expense, and it is difficult to prepare a full-scale specimen. On the other hand, numerical analysis for RC structures can reduce the number of experiments currently required and enable efficient design of structures and development of construction methods.

In this paper, an attempt is made to apply the American Society of Mechanical Engineers (ASME) standard ASME V&V 10 as a method for verification and validation (V&V) of computational models for RC structures, following the ASME procedures for computational verification of computational models and quantification of uncertainty of computational results. The reality of interest is an experiment conducted by Kurumatani et al. in which three RC beam specimens of the same specifications were subjected to flexural failure in five different organizations. The computational model used is a finite element method model with a smeared cracking model developed by Morikawa et al. The computational model is validated by probabilistic analysis considering the uncertainty of the computational model and input parameters. Finally, the prospects of V&V for actual structures are discussed.

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A two-stage method simulating random field over manifold

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Key Words: Random field, Manifold, Two-stage, geodesic distance, Isomap

Random fields are widely used to characterize spatial variablity. However, the common simulation methods are not suitable for manifold due to its complex correlation structure. This study introduces a two-stage method to simulate random fields over manifold. At the first stage, the manifold is transformed into a Euclidean domain by dimension reduction algorithm, then over the Euclidean domain the random field is generated by common existing methods at the second stage. The final random field over manifold is obtained by mapping the random field over Euclidean domain back to the manifold. The key of the two-stage method is the transformation at the first stage, where the correlation structure, which is evaluated by geodesic distance, needs to be preserved. Therefore, any dimension reduction algorithm preserving geodesic distance and common random field simulation method can be coupled into the two-stage method. In this study, we adopt the Isometric mapping (Isomap) with accurate geodesic distance as the dimension reduction algorithm and stochastic harmonic function representation as the common random field simulation. Several examples with random fields over manifold are demonstrated the applicability of the two-stage method.

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An Example of the Verification and Validation for Fracture Analysis of Reinforced Concrete Using a Damage Model

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Key Words: *Verification and Validation, Uncertainty, Reinforced Concrete, Damage Model*

An example of the verification and validation, based on ASME VV-10, for analysing reinforced concrete beams is introduced. The finite element method with non-linear material constitutive laws of concrete and steel is used for the computational model. A damage model based on fracture mechanics of concrete [1] is applied to the analysis of crack generation and propagation in concrete. The quantification of uncertainty about material properties of concrete is also performed in the validation of the computational model.

We first show our computational model [1], used in the verification and validation, for the non-linear analysis of reinforced concrete. The model is based on the finite element method with non-linear material constitutive laws. The modified von-Mises damage model is applied to concrete, and the standard von-Mises plasticity model is applied to steel. Finite element meshes of reinforced concrete beam reflecting the geometry of deformed bars are prepared in 3D.

An example of the verification is second presented. A model based on Euler- Bernoulli beam theory with material non-linearity is used for the verification, and the results are compared to the numerical results obtained from the 3D finite element analysis. From these results we confirm that the load-displacement responses conform to the reference solution of beam theory without the dependence of mesh-size.

We finally show a validation example along with the uncertainty quantification. The variation of material properties in concrete is regarded as the uncertainty in both the simulation and experiment in this study. A series of numerical result obtained from Monte Carlo simulation is compared to a series of experimental results obtained for quantifying the uncertainty of reinforced concrete beams. Good agreements are found between the numerical and experimental results, implying that the computational model is validated for the intended use.

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Application of Non-Linear Stochastic Finite Element Method based on Multi-Element Non-Intrusive Spectral Projection Method to Stochastic Elasto-Plastic Problems

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Key Words: *Intrusive Spectral Stochastic Finite Element Method, elasto-plastic problem, Non-Intrusive Spectral Projection, Multi-Element Polynomial Chaos*

In this talk, I will summarize the recent activities focused on the application of the intrusive Spectral Stochastic Finite Element Method (intrusive SSFEM) [1] to probabilistic elasto-plastic solid mechanics. Compared to Monte Carlo simulations, which require thousands or tens of thousands of calculations with varying parameter values, the intrusive SSFEM is very attractive because, depending on how it is used, all the necessary probability moments can be obtained in one calculation. The objective of this research is to develop the intrusive SSFEM that can be applied to solve probabilistic elasto-plastic solid mechanics problems. In general, however, the following two problems are obstacles to this goal. (1) the problem of the stress return mapping algorithm in a probability space, and (2) the problem of the very complex process of constructing stochastic matrix equations by applying polynomial chaos expansion (PC exp.) to the tangential stiffness and internal force stochastic matrices. The problem (1) implies that it is difficult to find the exact probability distribution of the yield function that is updated by the return mapping. And finding a stochastic stress field that accurately reflects that probability distribution is the bottleneck. The next 2) is the problem that existing non-linear FEM programs cannot be used as-is because all random variables such as displacements, strains, stresses, and stiffness matrices need to be decomposed using perturbation method or spectral expansions method when constructing the tool. In order to solve the problems (1) and (2), I developed a method called NISP-SSFEM, which is a combination of the non-intrusive spectral projection method (NISP method) and the intrusive SSFEM. NISP-SSFEM is a hybrid method to overcome the problems (1) and (2), where the NISP method is used to update the stress in a probability space and calculate the stochastic stiffness matrix and stochastic internal force matrix of the element, and the intrusive SSFEM is used to solve the global stiffness stochastic matrix. Then, a powerful method developed by Wan and Karniadakis[2], multi-element PC exp., is incorporated into NISP-SSFEM to solve the problem of instability caused by the setting of the number of numerical integration points in stochastic projection. In this presentation, I will introduce the multi-element NISP-SSFEM and conduct numerical experiments to evaluate this method by comparing the results with those of Monte Carlo simulations.

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Decoupled Multiscale Damage/Strength Analysis of CFRP Laminates

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Key Words: *CFRP, Laminate, Damage, Strength, Multiscale, Homogenization*

Carbon fiber-reinforced plastic (CFRP) laminates are materials manufactured by stacking prepregs (laminae) made of resins reinforced with carbon fibers. They have excellent characteristics such as light weight, high specific rigidity and strength, and they are used as structural members in a wide range of industrial fields such as aerospace, automotive, and energy industries. For CFRP laminates, it is known that damages in the micro-scale can lead to macro-scale failure. Therefore, it is very important to analyze the damage initiation and damage propagation behavior in CFRP structural members.

An effective method for structural analysis of CFRP laminates is the two-scale analysis method based on a homogenization theory [1, 2]. This method is able to simultaneously analyze the micro-behavior inside the material and the macro-behavior of the entire structure. The method therefore can precisely analyze the damage/strength of CFRP structural members. However, computational costs of the method generally become quite high.

In this study, we develop a decoupled multiscale damage/strength analysis method for CFRP laminates that provides high efficiency by analyzing micro and macro damage behaviors separately. For this, the Hoffman criterion is introduced into unit cell analysis, and macroscopic behavior and strength of a unidirectional CFRP (lamina) are obtained through coupled multiscale analysis based on the homogenization theory. Then, macroscopic constitutive equations that reproduce the obtained macroscopic behavior and strength are developed and incorporated into commercial finite element analysis software. Using the developed method, damage/strength analysis of CFRP laminates is performed, showing that the method can efficiently analyze damage/strength behaivor of CFRP laminates.

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Downscaling biomechanics simulation of mandibular bone from macroscopic oral implant to nanoscopic osteon using micro-CT and SHG images

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Key Words: *Bone biomechanics, Collagen, Image-based analysis, Zooming FEM, Arbitrary load*

In the field of bone biomechanics, micro-CT image-based analyses have been widely used including the direct modelling of porous trabecular bone. Recently, a new imaging apparatus, second harmonic generation (SHG) technique, has been developed that provides us with nanoscopic information of collagen. When it is applied to the bone, the osteon is visible, and many histological studies have been reported so far. However, as far as the authors know, no report is found on the SHG image-based finite element analysis except our previous report[1]. A novel biomechanics simulation of osteon that is consisted of collagen lamella surrounding blood vessel is expected to give new insight into the study on osseointegration.

The purpose of this study is to analyse the strain in collagen fibres in osteon near the oral implant under the loading condition applied to the implant. The oral implant can be modelled by the micro-CT images for a cadaver. To connect the macroscopic implant and nanoscopic osteon, a traditional zooming finite element modelling was used. The resolution of micro-CT images in this study is 90 μm, and that of SHG images is 0.83 μm, which is accurate enough to model 300 μm square region covering an osteon. The voxel finite elements were used with the same size with the resolution. To bridge the macroscopic and nanoscopic finite element models, a mesoscopic model with 9 μm mesh size was used. The zooming analyses were basically done by customized commercial software VOXELCON (Quint Corp., Tokyo, Japan) and controlled by in-house python code.

In the linear elastic finite element analysis, to consider arbitrary loading condition for two oral implants, the displacements under unit loading conditions were analysed first and stored in the database. In this report, we compared the strain distributions obtained under different loading conditions.

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Effect of material properties of pedicle screw fixation system rods on surgical treatment of kyphosis using patient specific finite element models

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Key Words: *Biomechanics, Finite element method, Computer-aided engineering, Lumbar kyphosis.*

The number of degenerative spine disease patients and the portion of lumbar kyphosis are growing. However, biomechanical researches on kyphosis and its treatment are scarce. In this study, the characteristic effects on kyphosis and the influence of material properties of treatment device were investigated in the view of biomechanical behaviours. The finite element method and statistical analysis were adopted for the study. Fourteen patient-specific finite element models were constructed from patients. To investigate the biomechanical influence of material properties of pedicle screw fixation system rod and bone graft cage, different material properties of rod and cage were incorporated in the finite element models. Three materials were adopted for connecting rods to analyse the influence of material properties. For loading conditions in finite element analysis, the vertical load of 400N and moments of 7.5Nm were applied for muscle force and 4 representative spine motions. From the biomechanical point of view, five parameters, intradiscal pressure(IDP), range of motion(ROM), anterior disc height(ADH), and posterior disc height(PDH), von-Mises stress of bone graft were analysed statistically to clarify the characteristic effects on kyphosis and influences of material property of connecting rod. The parameters were compared between the normal and patient subjects and different material properties of connecting rod. The ADH of kyphosis patients shown significant decrease compared to those of normal subjects. The PDH of L3-L4 in patients shown significant decrease. Statistically, the ROM and IDP of patients were decreased significantly. The von-Mises stress of bone graft was the maximum in patients treated with connecting rod using PEEK. The IDP of the adjacent segment was minimum when PEEK was used for connecting rod. The ROM of subjects was maximum when PEEK was used for connecting rod. The discussed results in this study will be important for the research and treatment of lumbar kyphosis.

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Gaussian Process Regression Surrogate Modeling with Transfer Learning for Low Computational Cost Structural Reliability Analysis

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Key Words: *Surrogate Model, Transfer Learning, ARD Kernel, Gaussian Process Regression*

Monte Carlo simulation is often adopted for the structural reliability analysis of civil structures that considers the parameter uncertainties, such as uncertainties of structural properties and input loads in the structural analysis. However, as the uncertain parameters become higher dimensional, the number of samples required for probability convergence increases, which increases the computational cost. To reduce the computational cost, the use of surrogate model was shown to be effective in many previous studies. However, most of these models are trained only for the target task. The surrogate model trained for the specific task cannot contribute to the reduction of the number of training data in constructing the surrogate models for other tasks.
In this study, we present a Transfer learned Gaussian Process Regression Surrogate Model (TF-GPRSM) for structural reliability analysis. Transfer learning has recently attracted much attention in the field of machine learning, where the knowledge gained from a model built for one task can be used to build a model for another task. There are a few previous studies that use the transfer learning for the surrogate modelling. For instance, Tian et al [1] used the transfer learning in the deep neural network in the idea of Variable Fidelity Surrogate Model (VFSM). It was shown that the constructed surrogate model could reduce the computational cost of analysing a fine-mesh FE model. In this study, we aim to reduce the computational cost by using the transfer learning to build the surrogate model for the structural analysis in the reliability analysis. Here, the ARD (Automatic Relevance Determination) kernel is used for the Gaussian process regression. By using the ARD, the contribution of each uncertain parameter to the output response can be determined, and those contributions can be used to evaluate the similarity between the original task and the purpose task in the transfer learning. The TF-GPRSM was evaluated for two verification cases. One is the case for the seismic performance evaluation of a bridge pier structure considering the variation of earthquake load. Here, the TF-GPRSM was applied to the surrogate modelling of the nonlinear time-history analysis of a lumped-mass model of the seismic isolated bridge pier. The inputs of the surrogate model were structural property uncertainties and the outputs were the maximum displacements of the seismic isolation bearing and the pier for the evaluation. A pre-built model with one earthquake load was transfer trained to a surrogate model with another earthquake load. The other case was the live load capacity analysis of a steel plate-girder bridge considering the uncertainties of damage conditions using the FE model. In this surrogate model, the inputs were structural properties including the parameters to represent corrosion damages, and the output was the maximum Mises stress at the steel girders. A surrogate model was built beforehand in the undamaged state, and the information from that model was used to build a surrogate model using transfer learning for the model after damage. In both cases, the models with and without the transfer learning were compared by verifying the accuracy and the cumulative distributions of the outputs for the structural reliability analysis. As a result, it was shown that the TF-GPRSM could predict the outputs with higher accuracies, and the number of training data required to obtain the same regression accuracies could be significantly reduced.

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High Quantile Estimation for Transpiration Cooling

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Key Words: Error Estimation, Quantile Estimation, Surrogate Modeling, Uncertainty Quantification, Transpiration Cooling

Transpiration cooling is a promising cooling technique aiming to enable safe operation in applications as e.g. rocket combustion chambers, where the material will not withhold the temperatures by itself. Incorporating parameteric uncertainties into the model leads to stochastic outputs of the system, e.g. the temperature is a random variable. In the area of quantile estimation, reliable methods are explored that efficiently evaluate high quantiles for the purpose of risk assessment, reliability and decision analysis [1].

In this talk, a novel approach is introduced that identifies the unknown quantile of the hot gas temperature using an empirical distribution system [2] which statistical properties are extracted by generalized Polynomial Chaos (gPC) expansions. The method is tested on a transpiration cooling model which consists of an one-dimensional model for the flow through the porous medium and a two-dimensional Reynolds-averaged Navier-Stokes model for the hot gas flow in a rocket combustion chamber, where the two domains exchange boundary conditions at the interface [3].

An error analysis of the suggested method is proposed which allows assessing the necessary accuracy of the gPC meta-model. Another advantage lies in the closed form expression of the quantile which makes directly integrating the risk assessment into an optimization context suitable. Additionally, an analysis of the numerical results shows the decreased computational expense due to meta-model techniques and various contributions of the method to risk assessment for transpiration cooling in the bigger picture of rocket combustion chambers.

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Multiscale Inelastic Analysis of FW-CFRP for High-Pressure Hydrogen Tanks

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Key Words: *Filament Winding, CFRP, Hydrogen Storage Vessel, Homogenization.*

Recently, fuel cell vehicles (FCVs) have been attracting attention due to their low enviromental impact. FCVs need high-pressure hydrogen storage vessels (hydrogen tanks), and carbon fiber-reinforced plastics (CFRP) are applied to the tanks because of their lightweight and high strength.

The filament winding (FW) method is generally used to manufacture CFRP hydrogen tanks. In this method, fiber bundles are wound in the hoop direction and helical direction to cover the curved surfaces of hydrogen tanks, and the stiffness and strength are controlled by the way of winding. Therefore, it is important to analyze the effects of fiber bundle orientation angles and winding misalignment on the mechanical behavior of CFRP manufactured by the FW method (FW-CFRP).

The mathematical homogenization method, which can analyze macroscopic and microscopic properties of heterogeneous materials, is one of the most effective methods for such analysis. In fact, the homogenization method has been developed into a form applicable to time-dependent deformation problems [1], and elastic-viscoplastic analysis of textile composites with consideration of laminate misalignment has been performed [2]. However, the homogenization analysis method for FW-CFRP has not been established yet.

In this study, elastic-viscoplastic behavior of FW-CFRP for hydrogen tanks is analyzed based on the homogenization method. For this purpose, three-scale elastic-viscoplastic homogenization method for FW-CFRP is proposed to consider macro/meso/micro behaviors of FW-CFRP simultaneously. Then, a unit cell modeling method for FW-CFRP with various fiber bundle orientation angles and winding misalignment is established.

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Numerical prediction of misorientation of drilling during oral implant surgery considering morphology of mandibular trabecular bone and study on drilling force sensing

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Key Words: *Computational biomechanics, Oral implant surgery, Trabecular bone, Morphology, Homogenization analysis*

The oral implant is now often used in dental treatment, but accidental cases still happen due to the lack of skill and experience of surgen, -by giving damage to nerve system in mandibular canal or to blood vessel after perforating lingual cortical bone during drilling jaw bone in the implant surgery. With this background, in order to contribute to the dental education, the authors have developed a drilling force sensing device [1] together with a stochastic finite element modelling method to calculate the drilling force considering inter-individual differences [2]. The stochasic computational method employed the first-order perturbation based stochastic homogenization method and uncertainty modelling method in micro-CT image processing, and a correction factor was calibrated by many experimentally obtained data for spine in others' published papers [3].

In the above-mentioned privious studies, it was assumed that the accidental case happens if the drilling direction was originally wrong. On the other hand, this study studied on the untintentional misorientation during drilling, even if the original directdion was correct, due to the nature of the microsocpic morphology in the trabecular bone region. By analyzing a 4 mm cubic representative volume element at the tip of the drill by the asymptotic homogenization method, sudden change in the orthotropic characteristics due to the micro-architecture has been found. Assuming this can cause the unintentional shift of the drilling direction, we compared the drilling forces between two cases with and without misorientation. They were also implemented in the force sensing device. In the virtual experience of two cases, the difference in force was clearly detected.

In this study, the bone volume fraction was compared with the predicted drilling force, which could explain partially the drilling force. However, the morphology analysis by the homogenization method could predict the possibility of misorientation.

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Numerical study of orthopaedic implant surgery for the development of stability evaluation device with consideration of uncertainties

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Key Words: *Computational biomechanics, Implant stability, Uncertainty modelling, Bone-screw interface, Laser pulse, transient response analysis*

In the orthopaedic treatment using implant for acetabular cup [1] or spine [2], the stability of the screw must be assured during the surgery. A torque meter has been used, but a new non-contact type device using laser resonance frequency analysis has advantages similarly to Osstell [3] that is available for smaller sized dental implant than orthopaedic implant. Supported by AMED (Contract number: 20hm0102077h001, 2020-2023), a prototype apparatus has been developed and applied to polyurethane forms simulating human trabecular bone. The measured insertion torque and pull-out force had a strong correlation. However, when the peak frequency was compared with them, it was hard to identify insertion torque and pull-out force from the peak frequency. This was because the peak frequency showed variability for a certain insertion torque as well as a certain pull-out force. Therefore, in the clinical use for living patients, larger variability will be included in the measured data. This motivated us to study on the uncertainty factors and perform probabilistic simulation.

The transient response was analysed for a cubic model consisting of cortical bone surface layer and trabecular bone region under laser pulse excitation considering three main uncertainty factors. The first one is the thickness of the cortical bone layer. The second is the size and the mechanical properties of the bone-screw interface. The third factor may lie in the laser pulse applied by surgeon. Concerning the thickness of the cortical bone layer and the radius of bone-screw interface, 3 geometrical random parameters were defined. To define the physical random parameters, the trabecular bone in the bone-screw interface region was subdivided into 4 sections, and totally 5 parameters were defined including the cortical bone. For the modelling of laser pulse excitation, two angles and two positions were considered as the uncertainty parameters.

To reduce the computational cost for the transient response analysis by finite element method, the eigenvalue analyses were carried out for 256 cases to evaluate the influence of geometrical and physical random parameters on the eigenvalues. The combination of random parameters was narrowed down to 10. Next, the transient response analyses were performed by adding 6 loading conditions, and obtained the probable variability in the peak frequency. Note that 10-node tetrahedral quadratic element and COMSOL Multiphysics ver.5.6 were used for this study.

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Probabilistic modelling and homogenization analysis of porous support structure for titanium alloy additive manufacturing considering defects

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Key Words: *Additive manufacturing, Defect, Statistical measurement, Micro-CT, Probabilistic Modelling, Homogenization*

The metal additive manufacturing (AM) or 3D printing is becoming a matter of interest as a new manufacturing technique for light-weight or topology optimized components as well as patient-dependent medical devices. One of the problems in AM is the higher possibility of defects, geometrical imperfection and the variability in material properties. Another difficulty lies in the determination of the building direction and support structure. The support structure is consisted of porous micro-architecture, which includes some design parameters. The process simulation by finite element method (FEM) will be of great help to the design of support structure from macroscopic standpoint. However, the porous micro-architecture is not considered at this moment. For instance, the CAD data of the porous micro-architecture tells us that the mechanical properties such as the Young's modulus and the coefficient of heat conduction are orthotropic, but the current existing commercial process simulation tools assume the isotropic material model for the support structure, as far as the authors know.

A preliminary experimental study of ours told us the occurrence of cracks in the support structure during the manufacturing process was strongly dependent on the geometrical design parameter for the micro-architecture. This fact motivated us to investigate the microstructures by micro-CT, partially based on our previous study on the additive manufacturing of lattice components [1].

Many defects and the variability in strut widths were observed. 6 geometrical parameters to express the discontinuities of struts were defined and statistically measured using micro-CT images. Also, the distribution of strut widths was measured statistically. Next, 21 probabilistic microstructure models were generated for the homogenization analysis by FEM to calculate the expected values of the macroscopic mechanical properties and the coefficient of heat conduction as the equivalent orthotropic model. A commercial software VOXELCON (Quint Corp., Tokyo, Japan) was used for the homogenization analyses. The outcome of this study including both statistically measured data and the numerically predicted homogenized properties will contribute to more accurate process simulation for additive manufacturing.

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Probabilistic modelling of geometrical imperfection for additively manufactured circular hole using aluminum alloy and polyamide

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Key Words: *Additive manufacturing, Building direction, Geometrical accuracy, Probabilistic finite element modelling*

The additive manufacturing (AM) or 3D printing technology has been attracting attention in both industrial and medical fields. One of the disadvantages over conventional manufacturing methods such as milling and casting is the higher possibility of microscopic defects and macroscopic distortion of the products. The authors have studied on the geometrical accuracy or imperfection [1] and proposed a probabilistic finite element analysis based on the statistically measured database of geometrical parameters [2].

Another difficulty in AM lies in the determination of building direction and support structure. To achieve good geometrical accuracy, for instance when the product includes circular hole or cylinder part, the choice of building direction is very limited [3]. The authors have found the correlation between the distortion of a circular hole in a flat plate and the building direction in the case of selective laser melting (SLM) of polyamid-12, PA2200 [4]. This study revealed that the proposed methodology to describe the correlation between specific geometrical parameters for distorted circular hole and the building direction holds also for aluminum alloy (Al-Si10-Mg). The constructed database enabled us to predict the mechanical behavior by finite element analyses of a product with a circular hole in a probabilistic way before manufacturing. Also the influence of the geometrical imperfection on the mechanical behavior of the product and that of the variability in material properties are quantitatively compared.

Finally, this paper proposed a design scheme to achieve a perfect circular hole by SLM of aluminum alloy for arbitrary building direction. To this end, the building direction can be determined without any limitation due to the circular hole.

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Quantification of the contribution of particle size distribution in granular flows

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Key Words: *DEM, Particle size distribution, Granular flow, Segregation*

The discrete element method [1] is well recognised as a powerful numerical tool of granular flow simulations. In DEM simulations, however, monodisperse granular models have been widely employed to reduce computation costs while the particle size distribution is one of the important factors controlling the flow characteristics. As a result, the effects of the particle size distribution on granular flow simulations have not been sufficiently studied.

The objectives of this study are to quantify the contribution of the particle size distribution on granular flows and to discuss the mechanism of its effect. A series of DEM granular flow simulation with different particle size distributions were conducted and analysed to investigate a relation between the particle size distribution and flow behaviour. A commercial software, which can solve contact problems of polyhedral objects with the help of the concept of the common plane [2], is employed for efficient numerical simulations. The obtained results clearly indicate that the run-out distance strongly depends on the number of particle sizes and is underestimated in the conditions employed by the monodisperse granular model. The longest run-out distance was recorded by the bidisperse granular model, whereas a constant value was achieved when the polydisperse granular models were employed.

Because particle size segregation was observed during the flow, a series of vibration simulations was also performed to estimate the degree of size segregation. It was shown that each granular model has its own inherent degree of size segregation. From the results of the presented granular flow simulations and vibration simulations, it is reasonable to conclude that the run-out distance has a strong correlation with the degree of size segregation.

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Sintering Simulation for Ceramics based on Multiplicative Decomposition of Thermo-Mechanical Deformation Gradient

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Key Words: *Thermal–Structural Simulation, Large Deformation, Ceramics, Sintering, Firing, Viscoplasticity, Master Sintering Curve*

Some simulation models have been proposed to predict the time evolution in the deformation of ceramics during the sintering process. Most of them link the thermal history and the sintering shrinkage by so-called “sintering stress” [1], but we would like to obtain the thermal deformation directly from the thermal history. In addition, since the temperature gradients occur inside the structure during heating, it is better to employ a unified model independently on the temperature histories to represent the thermal deformations.

We propose a simple strategy for the sintering simulation with Master Sintering Curve (MSC) [2], which considers microscopic thermodynamics from a macroscopic perspective [3]. In this simulation models, the deformation gradient is multiplicatively decomposed into thermal and mechanical component, and they are further divided into reversible and irreversible component. Assuming that the mechanical and thermal deformations are independent, each deformation component is determined by referring the experimental results of the time evolution in the deformation with/without uniaxial compression loads. The thermal and mechanical reversible deformations are represented by the commonly accepted models, namely thermal expansion and Hencky model [4]. MSC is employed for the thermal irreversible deformation (sintering deformation). It shows a density evolution from any temperature histories and it is easily obtained by sintering experiments. For the mechanical irreversible deformation, the viscoplasticity model [4] is used to represent the creep deformation during the sintering process.

The sintering simulation is performed by installing the model with User Programmable Feature (UPF) into ANSYS thermal–structural analysis. The simulations are validated by comparing with experiments on the time evolution in the deformation. Using this simulation, we would clarify the effects on the total deformations and the stresses of the temperature distribution during the sintering process and the internal heterogeneity.

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Two-Scale Damage Propagation/Strength Analysis of CFRP Laminates Considering Variability of Fiber Strength

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Key Words: *CFRP, Damage, Strength, Variability, Multiscale, Homogenization*

Carbon fiber-reinforced plastic (CFRP) laminates are important materials especcialy in aerospace and automotive industries because they have high specific strength and stiffness. Failure of structural members made of CFRP laminates is caused by damages in the micro-scale such as matrix cracking and fiber breakage. It is therefore necessary to analyze macroscopic and microscopic damage behaviors of CFRP laminates simultaneously.

For such multiscale analysis, the two-scale analysis method [1] based on a homogenization theory is one of the most useful methods. Using the two-scale analysis method, the macroscopic and microscopic behaviors of CFRP laminates can be accurately analyzed at the same time. Therefore, this research group has developed a two-scale analysis method applicable to damage propagation and strength analysis of CFRP laminates [2]. In this analysis, however, all fibers were considered to have the same tensile strength, and it was not possible to take into account the effects of fiber strength variability obserbed in actual CFRP laminates.

In this study, a two-scale damage propagation analysis method is used to analyze the damage propagation/strength of CFRP laminates considering variability of fiber strength. The Weibull failure criterion is applied to carbon fibers, while the Hoffman rule is used for resins as a damage criterion. Damage propagation and strength of CFRP laminates under uniaxial tension are analyzed with and without considering the fiber strength variability. By comparing both results, effects of the fiber strength variability on the damage propagation/strength of CFRP laminates are investigated. It is confirmed that the fiber fracture occurs almost simultaneously when the variability of fiber strength is not taken into account, whereas it occurs gradually when the variability of fiber strength is considered.

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Uncertainty Quantification and Validation in Failure Simulation of Reinforced Concrete Using Discrete Element Model

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Key Words: *UQ, Validation, Reinforced concrete, Failure simulation, RBSM*

Failure simulations of reinforced concrete members using Rigid-Body-Spring Model (RBSM) [1][2][3] are carried out as a case study for validation including uncertainty quantification of simulation based on ASME V&V guidelines. The experiment of interest is a flexural shear loading test of a reinforced concrete beam, in which 15 specimens were tested under same conditions. The validity of the simulation model is confirmed by comparing the mean and variation of the response values. The results of the study show that the method considering uncertainty quantification is more costly but more explicit in assessing the accuracy of the model compared to traditional validation methods.

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"This One Weird Trick to Put Error Bars on Molecular Simulations, Statisticians Love It!"

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Key Words: *Molecular simulation, transport coefficients, uncertainty quantification, statistics*

Molecular-dynamics (MD) simulation is a standard tool in the toolkit of a modern computational mechanician and is used to compute all kinds of properties of science and engineering interest. Despite the ubiquitous use of MD simulations, a task as nominally simple as computing an error bar to place on a measurement can be laden with subtleties. As MD simulation continues to grow in popularity, as advances in hardware and software enable unprecedentedly large and long MD simulations, and as data-driven techniques increasingly demand large datasets produced using this technique, it is critical that the molecular simulation community prioritizes rigorous statistical quantification of uncertainties associated with MD simulations.

In this talk, we present results on a simple yet illustrative vignette that demonstrates the power of a rigorous statistical approach, namely, computing the (self-) diffusion coefficient in a variety of fluid and soft-matter systems, ranging from the ideal to the (fairly) realistic. In each case, we show that commonplace techniques for estimating standard errors in diffusivity measurements (used essentially universally throughout the literature), frequently generate overconfident estimates of this transport quantity. In each case, we identify the core statistical assumptions that plague the standard approach, leading to this overconfidence. We conclude by presenting a simple scheme, inspired by a time-series analysis technique initially developed by econometricians, that enables accurate quantification of uncertainty in diffusion for fluids and soft-matter systems.

Finite Element Analysis at Pin Joints of Modular Bridge under Uniaxial Tensile Loads

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Key Words: *Modular Bridge, Bailey Bridge, Pin Joint, Joint Strength*

Modular bridges can be constructed in a short time by combining standardized rectangular panels according to the site conditions. They are mainly used as temporary or emergency bridges owing to reduction of the construction time by their pin joints. A Bailey Bridge is a typical modular bridge developed by D. Bailey in 1943 during World War II. Its standard panel consists of a rectangular framed panel (width 3048mm and height 1448mm) with a truss structure. The panel have four pin joints at its corners: two male and female types of the pin joints at the left side and right corners on the panel. The joints are completed by inserting steel pins (diameter 48mm) into the interlocking parts. Most of the studies on the modular bridges focused on the strength and layout of the panels [1, 2], and there was a limited knowledge on the pin joints. Hence this study focused on the pin joint of the Bailey Bridge and clarified the influence of its shape to the joint strength by numerical FE analysis.

Parametric analysis was conducted in order to investigate the effect of pin joint specifications on the strength under uniaxial tension loads. A partial model based on the pint joint of the Bailey Bridge was considered, and eight numerical cases were set up by difference design parameters, that is, the pin diameter, joint shape, and the diameter gap between pin and pin hole at the pin joint. For the pin diameter (3 patterns), the size of the pin in each case was determined by the ratio of the diameter to the distance from the centre of the pin hole to the edge of the pin joint. For the joint geometry (3 patterns), the number of teeth and thickness of the joint in the meshing area were varied. For the diameter gap (1 pattern), the size of the gap was determined according to the limitation of the specifications for highway bridges in Japan.

The pin joint strength under uniaxial tension was affected by yielding preceding either the pin, the area near the pin hole, or the other member. The pin joint of the Bailey Bridge yielded from the pin. As far as in this study, increase of pin joint strength of 18% was observed when the pin diameter was increased by 9mm compared to the Bailey Bridge model. It was also found that the joint performance was degraded by the gap between the pin and the pin hole of the pin joint.

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Bridge Modal Measurement Using a Novel Frequency-Free Test Vehicle in Parked State: Theory and Experiment

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Key Words: *bridge modal parameters, test vehicle, frequency-free, design, vehicle scanning method, vehicle-bridge interaction*

Abstract. In the application of the vehicle scanning method for bridges, the two factors of vehicle frequency and pavement roughness cannot be ignored. To tackle these at once, this study proposes the novel idea of designing and using a frequency-free test vehicle in parked *state* to retrieve the dynamic characteristics of the bridge. A single-axle test vehicle is considered frequency-free if its frequency is designed far larger than those of the bridges of interest. The test vehicle will also be free of pavement roughness if it is used in the parked (non-moving) state. Firstly, based on the bridge-vehicle transmissibility, it was theoretically shown to be feasible that a test vehicle can be designed to have a frequency far beyond those of the bridges of concern, while the spectral bridge frequency peaks will also be enhanced. Secondly, lab tests were conducted for the axle-wheel assemblies with inflatable or PU tires under ambient vibration. Of interest is that the axle with PU tires shows a favorable *random*, *small* and *even* spectral distribution with no self frequency up to 20 Hz. The PU tires was then assembled as a part of the test vehicle that is self balanced in entity. Finally, the self-made test vehicle was calibrated on a benchmarked bridge and applied to the Xiamen Bus Rapid Transit system. Taking a three-span girder bridge of the system as an example, it was demonstrated that the modal parameters (frequencies, mode shapes and damping ratios) of the first four modes of the bridge (flexural or torsional) can be well detected by the developed frequency-free test vehicle. Compared with the direct measurement, the proposed technique is *equally accurate*, but *more competitive in efficiency and mobility*.

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Detecting Bridge's Frequencies by the Rocking Motion of a Moving Test Vehicle

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Abstract: A self-designed single-axle vehicle is used to detect the bridge frequencies from its rocking motion, caused by wheels moving over uneven surface. For a single-axle vehicle, in addition to vertical motion which is often investigated in previous studies, it also has rocking motion along the axle of the single-axle vehicle. The single-axle vehicle is modeled as a two-degree-of-freedom (DOF) system, unlike its previous single-DOF version, to include both rocking and vertical motions. For the model adopted, the technique for calculating the responses of the wheels' contact points (CPs) with the bridge are newly derived to eliminate the vertical frequency, and especially rocking frequency of the single-axle vehicle. In the flat road test, the vertical frequency of the test vehicle is identified from the average of the two wheel sensors responses, and rocking frequency from the angular response calculated. From the field test conducted on a two-span girder bridge, it is concluded that: (1) the newly derived procedure for the left and right CP responses of the single-axle vehicle is reliable for scanning the first few bridge frequencies, while removing vehicle's frequencies; (2) the CP responses perform better than the responses of the single-axle test vehicle itself, in that bridge frequencies become more outstanding in the CP responses; (3) rocking motion of the vehicle enables us to better interpret the scanned frequencies; and (4)a temporary parking is beneficial for identification of bridge higher modes in the measurement.

Key Words: *Bridge, contact point, frequency, rocking, single-axle vehicle, vehicle scanning method, wheel*

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Detection of bridge frequencies using passing vehicles

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Key Words: *Bridge health monitoring; indirect method; moving load; vehicle-bridge interaction*

Indirect bridge monitoring methods proposed by Yang et al. [1-3] can be used to obtain modal parameters by means of vehicles passing over bridges. The advantage of this type of measurement is that the sensors are not mounted directly onto the bridge, but instead on the moving vehicle. Numerous publications have been devoted to this issue in recent years. The long term monitoring and identification of dynamic characteristics of bridges is important for assessing the condition of civil engineering structures as in the case of early detection of damage. A single-axle vehicle was designed and built for the experimental verification of modal parameters both in laboratory conditions as well as on real suspended footbridges. This paper focuses on an experimental study of the feasibility of detecting the fundamental bridge frequency from the dynamic response of a vehicle passing over the bridge. It was found from both the analytical and experimental studies that the bridge frequency is included in and can be extracted from the vehicle acceleration spectrum. The dynamic response of the vehicle, which in turn serves as a receiver or scanner of the dynamic properties of the bridge based on simplified measurements is efficient.

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Identification of Bridge Damage Location utilizing Low-pass filtered Accelerations of Slow Moving Cars

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Key Words: *Vehicle-bridge interaction, Bridge damage location, Low-frequency vibration.*

Locating damage of bridge structures is an important issue for bridge maintenance. One of the most general methods is using the acceleration of the bridge with double integration to generate the bridge deflection time history. Then the generated deflection would be compared to the deflection of a healthy bridge to detect and locate potential damage. However, it might be hard to get the precise deflection because the noise in structural monitoring and non-zero velocity can result in drifting of deflection through the integration process. Besides, the ideal health condition of a bridge, especially for some old bridges, usually requires bridge-by-bridge model updating which can be rather time-consuming for engineering applications.

This study proposed a direct method to locate potential bridge damage with the acceleration of several moving vehicles based on characteristics of the vehicle-bridge interaction system. Low-pass filtered vehicle acceleration was utilized for damage location with several slow-moving vehicles. The function of vehicle acceleration was derived from equations of the vehicle-bridge interaction system and the elementary beam theory. The function was proved to be a sum of a quartic function, which is related to the macroscopic elastic deformation of the bridge, and the unknown road roughness. Therefore multiple vehicles, whose mass was different, were utilized to eliminate the interfere from road roughness. Then the damage location can be determined by comparing the monitored vehicle vibration acceleration and the theoretical quartic function. Finite element simulation and experiments were proposed for validation with simply supported beams.

Superiorities of the proposed method over the integration are 1) the direct processing of vehicle acceleration can avoid potential interference from noise with integration, and 2) the model updating procedure can be omitted. The theoretical function would be used to check the damage location where the property of the cross-section should be abnormal and perform a clear difference from the theoretical functional curve. This method was supposed to be time-efficient and could be widely used in engineering applications.

Identification of track/bridge frequencies and track modulus by a instrumented moving test vehicle

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Key Words: *contact point; dual-beam model; track modulus; moving vehicle; vehicle-track-bridge model; vehicle scanning method (VSM)*

A theory is presented for retrieving the track/bridge frequencies and track modulus from an instrumented vehicle moving over a dual-beam model to simulate the track-bridge system. The dual beams are connected by uniform spring-dashpot units to simulate the effects of sleepers and ballast, etc. Based on the dual-beam model, the response of the vehicle is firstly derived in closed form, along with that for the vehicle-track contact point. The dual frequencies solved relate to the track and bridge frequencies. Compared with the vehicle spectrum, the contact-point (CP) spectrum is superior in that it is free of the vehicle and driving frequencies. Using the first "plus" frequency of the dual-beam system, the track modulus can be computed by a simple formula. The proposed technique is numerically validated against the key parameters involved. It is concluded that: (1) the first "plus" frequency can be retrieved from the contact-point spectrum as an outstanding peak; (2) track irregularity has an adverse, but tolerable, effect on retrieval of track modulus; (3) as a trade-off between efficiency and accuracy, the vehicle is suggested to move at a moderate speed; and (4) the proposed technique may be affected by track damping, but remains good for tracks with infinite length.

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Vehicle-Bridge Interaction System with Non-Uniform Cross-Sections

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Key Words: *non-uniform beam; three-mass vehicle; vehicle-bridge interaction; pitching effect; pavement irregularity*

In the analysis of a vehicle-bridge interaction system, the bridge is often treated as the uniform beam for simplicity. As such, the present study proposes a non-uniform vehicle-bridge interaction system by incorporating a three-mass vehicle model in a non-uniform bridge. It is assumed that non-uniform beam elements are of constant width and varying depth. For clarity, both mass and stiffness matrices are re-formulated to comply with the finite element sign convention. In this study, the vehicle scanning method is first adopted to obtain the non-uniform bridge frequencies as the reference. Then, the parametric study is conducted to investigate the influences of associated parameters on the identification of bridge frequencies, including vehicle damping, bridge damping, and pavement irregularity. With the three-mass vehicle model, the desired accuracy subject to pavement irregularity can be reached.

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A computational framework for modeling discontinuities in anisotropic rods

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Key Words: *Anisotropic rods, large deformations, multi-stability, discontinuities.*

Anisotropic rods with irregular shapes, arbitrary distribution of material properties and orientation, and kinks and creases, are common in engineering applications including deployable grid shells, collapsible origami and kirigami rings, morphable robots, and stretchable electronics. In this contribution we present a computational framework that can be used for the modeling of anisotropic rods with arbitrary and discontinuous mechanical and geometrical properties undergoing large deformations. These elements are subjected to states of self-stress produced by inelastic strain. Arbitrary and discontinuous mechanical and geometrical properties of the rod are described by a unique continuous and differentiable function defined over its entire length. This function is obtained by combining a series of Heaviside functions that are successively asymptotically approximated by continuous and arbitrarily differentiable functions. The mathematical description of the anisotropic rods consists of a set of differential equations that describe the elastic behaviour of the rod and a set of boundary conditions imposed at its two ends. We solve the resulting two-point boundary value problem by conducting numerical continuation with AUTO 07P to detect and track various bifurcations and folds [1].
We employ the presented framework to study the folding and multi-stable behaviours of elastic slender rods and polygonal frames having discontinuous orientation of the longitudinal axis (i.e. kinks and creases), arbitrary distribution of inelastic curvature, material parameters, and cross section orientation and size. The presented numerical results demonstrate the efficiency and convenience of this novel framework in unveiling the very rich bifurcations and stable branches that characterize the behaviours of these anisotropic rod elements. Comparisons with experimental results obtained from tabletop models are used to validate our numerical predictions.

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A numerical approach to the design of gridshells for WAAM

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Key Words: *Form Finding, Wire-and-Arc Additive Manufacturing, Funicular Analysis*

Among different Additive Manufacturing (AM) processes, Wire-and-Arc Additive Manufacturing (WAAM) results particularly suitable for applications in structural engineering. The WAAM process, which consists of off-the-shelf welding equipment mounted on top of a numerically controlled robotic arm, allows realizing large-scale structural elements up to few meters, with limited constraints in terms of forms and shapes. The WAAM technique employing "dot-by-dot" printed stainless steel rods is herein considered, see in particular investigations in [1].

Gridshells take their strength from their double curvature, being constructed from members that mainly undergo axial forces [2]. A numerical approach based on funicular analysis, see e.g. [3], is proposed to cope with the design of spatial truss networks fabricated by "dot-by-dot" WAAM. The equilibrium of funicular networks can be conveniently handled through the force density method, i.e. writing the problem in terms of the ratio of force to length in each branch of the network. As investigated in the literature for the case of vertical loads, independent sets of branches can be detected for networks with fixed plan geometry [4].

In this contribution, following [5], the minimization of the horizontal thrusts in networks with fixed plan geometry is stated both in terms of any independent subset of the force densities and in terms of the height of the restrained nodes. Local enforcements are formulated to prescribe lower and upper bounds for the vertical coordinates of the nodes, and to control the force densities in the branches. This allows also for a straightforward control of the length and maximum force magnitude in each branch. Constraints are such that sequential convex programming can be conveniently exploited to handle grids with general topology and boundary conditions.

Preliminary numerical simulations are shown concerning the optimal design of grid shells with minimum thrusts, under the combined effect of different sets of the above prescriptions. The ongoing research is mainly devoted towards endowing the design formulation with buckling constraints.

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A Very Simple Fully Nonlinear Shell Finite Element

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Key Words: *Computing Methods, Finite element method, shells, Kirchhoff-Love, Mindlin–Reissner.*

Finite Element Method is a numerical tool for solving partial differential equations in Engineering and Science. In solid mechanics, structural models such as shells, bars and others are developed to simplify the complexity of 3D-simulations. Shells are one of the most important models in solid mechanics since many structures in engineering may be associated with it. It may be adaptable to finite element usage, but some particularities must be watched. For instance, if not treated properly, it is known that very thin structures may have inconsistent results regarding rigidity (see [3]) (locking phenomena) and consequently results may be untrustworthy. In view of this, the study of this type of simulations (shells models in FEA) is fundamental in present times.

The current project aims to study and develop a new simple shell finite element based on hybrid shear rigid/flexible model (Kirchhoff-Love / Mindlin–Reissner) for reliable and efficient simulation of thin nonlinear structures. This new shell triangular element has been tested with 6 nodes and does not use Lagrange multipliers or penalty methods to guarantee displacement C^1 continuity between adjacent elements (as required by Kirchhoff-Love models) or for canceling the drilling rotation (as required in some Mindlin–Reissner models. See [2]). The DOF's are the displacements u at the six nodes and the incremental rotation parameter φ_Δ at mid-side nodes (parameter φ_Δ is properly explained in [5]). The incremental rotation parameters α_Δ (incremental Rodrigues's parameters) and consequently incremental rotation tensor Q at the mid-side nodes are internal degrees of freedom that are computed at element level by solving a simple set of equations. The displacements u are interpolated by quadratic polynomials from the nodal values as usual.

The present work may be interpreted as a continuation of previous studies developed by the group of study from Professor P. M. Pimenta and more references may be found in [1], [2], [4] and [6]. The current model is still under development and results are going to be presented in forthcoming work.

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Damaging Configurations in Arch Structures with Variable Curvature and Tapered Cross-section

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Key Words: *Arch, Damaging, Structural design, Structural mechanics, Damaged Arch Structures, Variable Curvature, Tapered Cross-section*

Arch structure is a widely used and important structure type all over the World. Due to its beautiful form and large spanning capacity, arch structure is widely used in bridges, tunnels and other buildings. Especially in recent decades, the large span space arch structure has a stage of development. The defects of arch structure, such as connection, material, fatigue, stress concentration and welding, will directly affect the safety of long-span structure. The study of the evolution of the damage in structures is a topic of interest since the antiquity. A well-done structural design should always account for the evolution of the damage in time, in particular if it can bring to a change in the static behaviour of the structure itself under different loading conditions [1-3].

In this paper a model for the calculation of localized damaged in arch structures is presented. In particular, using an analytical solution for the computation of the displacements filed and the consequent internal actions of very general arch shapes with variable curvature and tapered cross-section, the damage is modelled by localized depletion of the cross-sectional properties (inertia) in the different points along the arch axis. In particular, the depleted parameters are the cross-section and the bending stiffness of the arch. Finally, the model is applied to the study different configurations of the damage (localization of plastic hinges or different pattern of defects) and to consider the evolution of the damage in time.

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Discovering Reciprocal Tensegrities with Symmetric Connectivity

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Key Words: *Self-stressed Structures, Tensegrity, Graphic Statics, Reciprocal Diagrams*

Graphic statics is a compelling geometry-based approach to the conceptual design of structures in static equilibrium. It is based on two interrelated constructs, the form and the force diagrams, the first representing the geometry of a pin-jointed framework in static equilibrium and the second indicating the equilibrium of forces within the structure [1]. The relationship between these two diagrams allows simultaneous control of both the form and the forces within a given structure. In this way, it is possible to transform one of the diagrams and evaluate the resulting modification of the other. In recent years, generalized methods for the construction and transformation of vector-based 3D force diagrams of 3D self-stressed [2] and externally loaded pin-jointed frameworks in static equilibrium [3] have been introduced.

In the particular case that the form diagram of a self-stressed pin-jointed framework has an underlying planar graph, its corresponding force diagram is reciprocal and can be regarded itself as a self-stressed pin-jointed framework whose force diagram is the initial form diagram [2][3]. In this contribution, we present a new procedure for generating novel self-stressed, topologically symmetric 3D pin-jointed frameworks by manipulating the underlying graph of a given form diagram. The procedure consists of the following steps. For a generic self-stressed 3D pin-jointed framework (single-primal), its underlying graph is first transformed into a topologically symmetric planar graph by duplicating all edges and vertices. Then, the dual graph of this newly generated planar graph is constructed. Considering the nodal equilibrium of the single-primal and conforming to the topology of the dual graph, a 3D force diagram is assembled in which all elements are duplicated (double-dual). This 3D force diagram is itself a self-stressed, topologically symmetric pin-jointed framework. Its corresponding reciprocal diagram is again a self-stressed, topologically symmetric pin-jointed framework (double-primal) in which all the elements are also duplicated. Different transformations of the underlying graph of the single-primal lead to the construction of varying double-primal and double-primal configurations and thus distinct self-stress pin-jointed frameworks. The proposed procedure is exemplified with several case studies, starting from various classical tensegrity structures as single-primal configurations.

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Evaluation of Tensegrity-Like Units for Nonlinear Mechanical Metamaterials

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Key Words: Bistable Unit, Mechanical Metamaterials, Additive Manufacturing

In this work, we investigate the nonlinear response of mechanical metamaterials assembled from tensegrity-like repeating units. Tensegrity-like structures are frame structures whose geometry and connectivity reproduce those of tensegrity structures, thus conferring to them also a similar mechanical response. Differently from tensegrities, tensegrity-like structures do not have cable members or nodal pin connections, and they are not prestressed, therefore they can be easily fabricated in one piece by additive manufacturing methods. Tensegrity-like units for mechanical metamaterials were proposed in [1], as multistable lattices, and in [2], as failure-resistant lattices, which in both cases were realized by multiphoton lithography techniques. In [3], tensegrity-like units were fabricated by fused deposition modelling and tested in compression, highlighting a nonlinear snapping response. By observing that changes in the geometry of a unit can result in different nonlinear behaviours, such as stiffening, softening, snap-through and bistable responses, here we consider different tensegrity-like units and their assemblies to evaluate the mechanical response of possible nonlinear metamaterial designs.

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Evolution of Distribution Algorithm for Constrained Optimization in Structural Design

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Key Words: *Structural Optimization, Evolutionary algorithm, Statistics, Evolution of Distribution Algorithm, Structural Optimization*

Nowadays, the need to deal with limited resources together with the new discovered awareness of the human over-exploitation of the environment, has made the optimization a cutting edge topic both in scientific research and in the different professional fields [1, 2, 3, 4].
In this paper, a particular evolutionary optimization algorithm is presented: The Evolution of Distribution Algorithm (EDA). This type of algorithm has been developed to be used in search-based constrained optimization problems which are difficult and time-consuming to be solved by other general algorithms. Being an evolutionary algorithm, the main idea is to generate a population of solutions and evaluate the objective function to each one of them. Then, using the information obtained from the previous generations, the algorithm step-by-step will generate new populations that will tend to the best value of the objective function. In EDA, the population of solutions defines a probability density function (PDF) and, by integration, a cumulative density function (CDF), which is used for the generation of the next generation [1, 2, 3, 4].
In structural design optimization problem, it is very common that the best solution is very close to the constraint function. The main advantage of applying the EDA for constrained optimization problem is that each generation of solutions is obtained starting from a PDF that is defined on the whole domain. This means that, for each generation, the solutions have a probability to be on the unfeasible domain space, maintaining the information about the objective function in the evolution process. In the present research, an original EDA and related self-made code are presented together with a specific application to structural optimization problem, in order to show the effectiveness of the obtained results and to make a comparison with other evolutionary optimization algorithms.

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Experimental Investigation of the Static and Dynamic behaviors of 3D-Printed Shell Structures

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Key Words: *Multi-body Rope Approach, Shape Optimization, Vaults, Dynamic Behaviour of Shells, Digital Image Correlation, Fuse Deposition Modeling*

Over the last years, several optimization strategies were conducted to find the optimal shape minimazing internal stress or total weight (volume) of shallow grid shells and vaults [1]. In recent times, this structure typology gained a great importance among researchers and the scientific community for the renowed interest in the form-findind optimization of column-free space solution for large span roofing construnctions [1]. In the present paper, a form-finding of a shollow grid shells was introduced basing on the multy-body rope approach (MRA) for the definitions of vaults with optimized shape and different hole percentage. In order to obtain an experimental validation, a physical model was reproduced at the laboratory scale performing ad hoc measurements to compare the observed respect to the simulated behavior. A 3D printing procedure based on the Fuse Deposition Modeling (FDM) technique in polylactide (PLA) material was used to realize formworks of the cement based blocks of the scaled prototype [2-3]. Several statical and dynamic load configurations are investigated, collecting into a sensitivity analysis the parameters which mainly affect the structural behavior [4,5]. To simulate earthquake ground motion an assigned frequency range as dynamic input to the structure was provided by a shaking table [4]. Statycal and dynamic monitoring of the vault prototype was performed using 2 USB (2 Mpx – 165 Hz) and 4 GO-PRO full HD (8 Megapixel) frame rate 100 fps. DIC measurements were used in order to validate the vibration modes of the vault obtained by the dynamic simulations. Finally, some preliminary considerations of the dynamic response of the model were provided testing the robustness of the form-finding approach when horizontal load are taken into account.

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Finite Element Analysis of Load Capacity of Panel Bridge with Multi-Scissors Structure

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Key Words: *Panel Bridge, Scissors-type Bridge, Multi-Scissors structure*

Panel bridges, such as the Bailey Bridge, are well used as temporary bridges that can be joined and assembled on site from standardized components. However, they made of steel and lack portability. In order to improve a workerbility on-sites of these temporary bridge, a scissors-type bridge is proposed [1]. The scissors-type bridge, which is an application of a deployable mechanism, has the merit that the entire bridge can be expanded and stored by the partial control. Furthermore, the use of lightweight aluminum alloys enables erection by a small number of worker and provides excellent portability. However, the rigidity of the aluminum alloys is low in comparison with the steels. In this study, the multi-scissors panel is applied to the scissors-type bridge (Herein multi-scissors-type bridge) to increase the performance of the bridge keeping the lightweight. Here we clarify the load capacity of the multi-scissors-type bridge with the different panel layouts.

Although the mass of the panels of panel bridge has been reduced in anticipation of manually work, each panel still exceeds more than 200 kg [2]. A panel of the multi-scissors-type through bridge made of aluminum alloys was assumed with a height of 1.0m and width of 2.0m. Numerical FE analysis was performed under the both-end supports conditions with a concentrated load of maximally 100kN increasing linearly in 1 second at the middle of the bridge. The number of layers of the panel was varied from one to five. This numerical analysis was performed with the single panel model and four panel model.

The stiffness of the panels for both the single and four was increased lineally by the number of panel layer of the multi-scissors-type bridge. The stiffness of four panels was 2.2% of that of the single panel. Maximum Von Mises stresses under the loading were found at the pivot near the supports for the single panel and at the pivot near the loading position for the four panel, and both models yielded in these positions. Therefore, the effect of bending moment was increased by the increment of the bridge's span. The bending stress was approximately 80-90% higher than the axial stress at the yield positions for each model. Furthermore, the bending stress decreased with increasing number of layers of the bridge and was inversely related to its mass in the case of the single panel. These results indicated that the bending moment which is dominant sectional force of this bridge can be reduced by multiplexing of the scissors structure.

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FORENSIC EVALUATION OF HISTORIC SHELL STRUCTURE: DEVELOPMENT OF IN-SITU GEOMETRY

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Key Words: *concrete shell, historic structure, folded beam, hyperbolic paraboloid*

When completed in 1961, the roof of St. Charles Church became the largest unbalanced hyperbolic paraboloid structure in the world and the only shell structure in Spokane, WA [1]. Situated on an 8-acre site on the north side of the city, St. Charles is a modernist structure designed through partnership of Funk, Molander & Johnson and architect William C. James. This asymmetric structure spans over 27.5m (90ft) and utilizes folded edge beams that taper from 1067mm (42in) at the base to a 76.2mm (3in) thickness at the topmost edge using regular strength reinforcing steel and concrete. The novelty of the shell structure serves both architectural and structural design criteria by delivering a large, uninterrupted interior sanctuary space in materially and economically efficient manner.

Having previously completed an initial analysis of the structure [2], now, 60 years later, a complete structural forensic evaluation of the shell has been conducted using full point cloud laser scanning to generate a complete in-situ model. The geometry is analyzed and deflections are compared to original design and construction documents to facilitate repair and maintenance of this architecturally and historically significant structure. A full structural evaluation of the roof and connecting structure has been completed. The forensic survey shows minor shear cracks throughout the shell field and deterioration of the underside of the shell. However, deflection at each tip of the hyperbolic parabola is neglibible compared to the design – highlighting the robust geometric stiffness and apparent resiliency of the prestressing. Results of the current in-situ geometry are compared to the design geometry of original construction documents.

Ongoing work includes detailed CFD modeling to determine accurate wind loads as well as comparison of historical and current design standards.

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Multi-body Rope Approach for the Form-Finding of Shape Optimized Grid Shell Structures

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Key Words: *Gridshell, Form-finding, Conceptual Design, Multi-body Rope Approach D'Alembert Principle, Phyton code,*

Over the past decades, different approaches, physical and geometrical, were implemented to identify the optimal shape, reducing the internal stresses, of grid shells and vaults. As far as their original organic shape is concerned, the design of grid shell structures inspired architects and structural engineers in more than one way [1-5]. Along the history time, the solution of the structural form-finding buried its roots on the activity of scientists and designers. In the present paper, the original approach for the form-finding is proposed by the dynamic numerical simulation of hanging net, subjected to gravity load, over the time domain [4]. In particular, the adopted process for the definition of the structural shape is based on a multi-body rope approach (MRA) with masses connected by inextensible ropes characterized by a certain slack coefficient (*sc*) and by the degree of the constraint conditions [4]. The method, originally presented in [4], is here re-developed and extended employing a self-made code based on the dynamic equilibrium, ensured by the d'Alembert principle, of masses interconnected by rope elements in space-time domain. The equilibrium corresponding the optimized shape to be defined, is obtained through an iterative process in the falling masses connected by a net for the definition of the "catenary surface" coinciding with the best shape of the shell (form minimizing the bending moment). The implementation of the method is realized in Python in an interpreted high-level general-purpose programming language. The adopted design philosophy emphasizes the code readability by other languages with respect to the traditional model realized in Visual Nastran 4D. By the use of this code as well as its object-oriented architecture the MRA Python code will be linked to the Grasshopper environment for the direct visualization of the shapes and their fast-parametrization phase.

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Bayesian data-driven learning of industrial light weight structure design optimisation under uncertainty

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Key Words: Uncertainty Quantification, Design Under Uncertainty, Data Driven Learning, Aerospce, Dimension Reduction, Gaussian Process Regression, Vector-Valued Functions, Lightweight Structures

Data-driven learning in the context of design under uncertainty is associated with the challenge of creating optimal high-dimensional maps of input parameters to vector-valued output quantities. This work focuses on an approach of compressing multi-output vector data and modelling it within a Bayesian framework. Three models are compared, a brute force learning of all output vectors, learning of reduced dimensioned (compressed) approximation of the vector-valued output, and a compressed model with log standardisation applied. Gaussian process regression with an isotropic squared exponential kernel function is used to learn the maps [2]. Compression is applied using principle component analysis (PCA). Log transformation of the data is applied to reduce bias in the PCA. Both the compression and standardisation introduce uncertainty which is quantified and propagated through the models along with the mixed uncertainty of the vector-valued output.

The data-driven learning is performed with a practical high-dimensional industrial problem aimed at a specifically parametrized aircraft wing configuration. In short, the input is made up of ten parameters over 201 uniformly distributed design of experiment points. The target data are the responses at points along the wing span when it experiences prescribed loading conditions producing a 8556 dimensioned vector-valued output.

It is found that the compressed model is able to reduce computational expense by up to 98% while incurring an increase of 5% in the relative error compared to the brute force and standardised model, where the relative error is of the order $\times 10^{-4}$. The use of an isotropic kernel enables the creation of response surfaces for input parameters of interest while retaining information on the predictive uncertainty at every sampled point in the surface, this is important as this framework lays the foundation for further work into design optimisation under uncertainty [1]. The methods used here are not dependent on demonstration application, and can be applied to any high dimensional machine learning task.

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Damage modelling and detection in beams by Newton-Raphson method

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Key Words: *Vibration, Damage detection, Rotational spring, Dynamic stiffness matrix.*

The catastrophic failure of structures has the potential to cause loss of life and incur significant economic loss. To overcome this scenario, the vibrational characteristics of the structure can be used to understand the current and future performance. The use of such vibrational characteristics such as natural frequency to detect damage further overcomes the difficulties of inspection in inaccessible areas of the structure [1, 2].

To model the effect of damage on the natural frequencies of an Euler-Bernoulli beam the exact dynamic stiffness matrix [3] has been formulated for a beam fixed at both ends in which a crack is modelled by a rotational spring. The formulated matrix yields a transcendental eigenvalue problem for which the Newton-Raphson method has been applied to yield the natural frequencies and mode shapes for uncracked and cracked cases. The obtained reductions in natural frequencies of the proposed system, due to presence of the crack, closely match with newly derived analytical solutions for the various locations of the damage.

The use of the Newton-Raphson method enables a high level of computational efficiency to be achieved in solving this forward problem (i.e. the change in natural frequencies due to a crack with a particular location and severity). The accuracy achieved in the forward problem provides a strong basis for solving the inverse problem to determine the location and severity of cracks based on measured changes in the natural frequencies of real structures.

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Nonlinear Dynamic Characteristics and Resonant Actuation of Bi-stable Structures

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In the fields of morphing aircraft, flow control and energy harvesting, dynamic characteristics of the multi-stable structure provide an idea for realizing change of the structure shape. Nonlinearity and local stability of multi-stable structures provide potential benefits for morphing structures as no energy is required to hold each stable configuration. This paper presents the dynamic characteristics of bi-stable laminate, including the effects of geometric dimensions and boundary conditions. Numerical simulation is used to study the nonlinear dynamic characteristics of each configuration and dynamic response under different excitation levels. A resonance actuation strategy leading to snap-through of bistable structure is investigated, and the realization conditions of single well vibration and cross well vibration are determined.

Keywords – morphing structure, bi-stable composite laminate, nonlinear dynamics, resonant actuation

Postbuckling Optimization of Stiffened Panels via Topological Design

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Key Words: *Postbuckling Optimization, Stiffened Panels, Topology Optimization*

As one of the primary structural configurations in aircraft, stiffened panels are ubiquitous and play an important role in aerospace due to their high stiffness-to-weight and strength-to-weight ratios. However, their load-carrying capability is strongly influenced by buckling. Many efforts have been made by using optimization techniques to maximize the critical buckling load or minimize the mass with linear buckling constraints. However, it is well known that stiffened panels can carry loads several times higher than the critical buckling load. Therefore, stiffened panels might be able to be designed to work in the postbuckling field beyond the critical buckling load, offering significant potential for further structural weight reductions.

Topology optimization is one of the structural optimization methods with the greatest degree of design freedom. It can help to determine the best possible shapes and material distributions for the prescribed objective by redistributing material. The authors have recently demonstrated the feasibility of applying the level-set-based topology optimization method to simultaneously optimize the size, layout and topology of stiffened panels for linear buckling [1-3]. In this work, this method is extended to consider postbuckling. To the best of the authors' knowledge, this is the first investigation of the postbuckling optimization of stiffened panels via topological design. Specifically, the stiffened panel is discretized into plate elements. The thicknesses of the skin and stiffeners can be optimized. A control mesh is developed to manipulate stiffener layout, and correspondingly the free-form mesh deformation method is utilized to adjust the finite element mesh. The level set method is used to optimize the internal topologies of the stiffeners as well as the number of stiffeners. The iterative Newton-Raphson scheme with load or displacement control is used for finite element analysis, where a small imperfection in the form of the first linear buckling mode is imposed on the finite element model. Different indices, i.e., total reaction force under given displacements, in-plane displacement under given loads and out-of-plane displacement, are considered to assess the postbuckling performance of the stiffened panel. They are respectively optimized with a mass constraint. A semi-analytical sensitivity analysis is performed, and a gradient-based optimizer is used to solve the optimization problem. Numerical examples are used to demonstrate the application of the proposed method. Compared with the initial design, the postbuckling performance of the optimized stiffened panels is improved.

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Study on Improvement of Bending Strength of Thin-Walled Structures Composed of Sandwich Panels

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Key Words: *Sandwich Panel, Lattice, Bending Moment, Critical Angle, FEM*

In recent years, there has been an increasing demand for structures with lightweight and high-strength properties in order to reduce the consumption of raw materials and energy. One such structure is the sandwich panel. Sandwich panels are a type of composite structure consisting of a low-density, lightweight core with a thin faceplate bonded to the surface.

An example of a core used in sandwich panels is the lattice structure. It is a structure in which long and thin beams are arranged in a three-dimensional and periodic manner. In recent years, advances in additive manufacturing technology have made it relatively easy to fabricate lattice structures with fine beams of several hundred micrometers in diameter. Furthermore, the lattice structure has the advantage that the mechanical properties can be adjusted according to the purpose of use by changing the diameter of the beams and the shape of the core, and it is attracting attention as an advanced structure that plays a role in reducing the weight and increasing the strength of structures.

An open-section beam was adopted as the shape of the sandwich panel in this study. Open cross-section beams, such as U-shaped beams, are widely used in automobile bodies and buildings. Chen et al.[1] investigated the bending behavior of open beams in a continuum, including the prediction of the maximum bending moment and the effect of the direction of bending, using numerical simulation analysis with FEM. M.M. Pastor et al. [2] [3] investigated the effect of beam cross-section size on the bending behavior and the maximum bending moment of U-shaped beams in a continuum using experimental and numerical simulation analysis with FEM. However, there is no research report on the bending of open-section beams in sandwich panels.

In this study, the bending collapse behavior of U-shaped sandwich panel filled with lattice has been investigated by using FEM. In particular, the effects of geometric properties of lattice core and faceplate on the maximum bending moment and the critical angle were discussed. The existence of a lattice core could prevent the elastic buckling of the surrounding U-shaped plates, and enhance the maximum bending moment to the fully plastic moment of these plates. Based on numerical investigation, the mode map with relative thickness of the plate and the relative density of the lattice core as parameters was obtained.

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The ROM-driven optimization of composite laminated plates for buckling and postbuckling performances

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Key Words: Postbuckling optimization, Reduced-order model, composite laminated plates

Thin-walled composite laminated plates are commonly used as primary components in aeronautic and aerospace structures to bear the in-plane compression loads, benefiting from their high strength-to-weight and stiffness-to-weight ratios. When composite laminated plates under compression are allowed to continuously loaded into the moderately deep postbuckling regime, further weight savings can be achieved. The standard nonlinear finite element(FE) analysis combined with the Newton-Raphson technique and its variants, is the most common method for calculating the postbuckling response; however, the repeated solutions for large-scale FE models in each incremental-iterative step are extremely computationally expensive. Therefore, the standard finite element method is not suitable for the postbuckling optimization process, which requires the evaluation of the equilibrium path for each change in the design variables(e.g. lamination parameters), because a single run is too time consuming with current CPUs.

For this purpose, this work presents an efficient optimization scheme for the design of postbuckling behaviour of composite laminates. The reduced-order modeling method based on the Koiter perturbation theory, is developed to calculate the postbuckling behaviors of the composite laminated plate. The initial postbuckling response is represented by the nonlinear predictor solved by the reduced order model(ROM), while the deformations in the moderately deep postbuckling regime are obtained by applying the corrections under the design load. Five different indices, including the critical buckling load, the initial postbuckling stiffness, the stiffness residual, and the in-plane and out-of-plane deformations under the design load, are depicted to valuate the various postbuckling performances of the compressed plate. These postbuckling indices can be flexibly selected to be either the objective or the nonlinear constraints in the lamination optimization. The optimal algorithms are subsequently adopted to determine the lamination configuration for the most favorable postbuckling performance. The various composite laminated plates with the straight/curved fibers are studied under uniaxial and biaxial compression for different boundary conditions.

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A General Higher-Order Shell Theory for incompressible and anisotropic hyperelastic materials using Orthonormal Moving Frame: an application to Arterial Mechanics

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Key Words: Isotropic soft shell, anisotropic soft shell, analysis of arteries, layered shell structure

This study presents a general higher-order shell theory to analyze the large deformation of single or multi-layered shell structures made of isotropic or anisotropic incompressible hyperelastic materials. The salient feature of this shell is threefold: (i) this shell theory formulation has been done using an orthonormal moving frame (OMF) instead of the classical natural covariant frame, which makes the mathematical formulation relatively simpler even for very complex hyperelastic constitutive relation owing to the orthonormal nature of basis vectors; (ii) General-higher order nature of approximation through-thickness of the shell make it equipped to model the deformation of a thick shell as well as multi-layered shell, and at the same time it also removes thickness stretch associated numerical locking, and (iii) the constitutive relations of incompressible isotropic and anisotropic hyperelastic material, both stretch and invariant based, are considered eying application in the vascular mechanics. The displacement field of the line normal to the shell reference surface is approximated by general Legendre polynomials single layer shell and by Lagrange polynomial for multi-layered shell structure. Subsequently, the kinematics of the shell for orthonormal basis has been derived using the tools of *exterior calculus*. It has been shown by Arbind, Reddy, and Srinivasa in [1] that such a coordinate system makes it possible to represent kinematic quantities, *e.g.,* determinant of the deformation gradient, far more efficiently than the in the classical tensorial representation with covariant basis. This study can be regarded as an extension of [1] for incompressible and anisotropic softshell for more general interpolated shell geometry. Here, for a general shell surface geometry, the finite element formulation of the shell theory is presented, and further, the theory has been applied to large deformation analysis of human arteries, which can be considered as thick layered tubular shell, under internal pressure. The incompressibility constraint has been applied via the penalty method as well as the Lagrange multiplier method. For the post-buckling analysis, nonlinear finite element formulation has also been presented considering the arc-length method. Various numerical examples are presented to verify and validate the formulation presented in this study.

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A New Mixed FE-Formulation for Liquid Crystal Elastomer Films

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Key Words: Anisotropy, Finite Element Method, Variational Principle, Energy-Momentum Scheme.

Liquid crystal elastomers (LCEs) are soft materials, which are capable of large deformations induced by temperature changes and ultraviolet irradiation [1]. Therefore, since many years, these materials are under investigation in experimental researches as actuator materials. LCEs arise from a nematic polymer melt, consisting of long and flexible polymer chains as well as oriented and rigid rod-like molecules, the so-called mesogens, by crosslinking. After this process, the flow ability and the orientation of the mesogens is retained. To date, the alignment of LCEs is primarily achieved in thin films. When the orientational order in the film is lost due to temperature changes or ultraviolet irradiation, the LCE film is capable of length changes of 400 percent.
In order to numerically simulate LCE materials as actuators in multibody system models by using the finite element method, a continuum formulation is necessary, which include in a thermo-viscoelastic material formulation of the polymer chains the orientation effects of the mesogens. This can be performed by introducing a normalized direction vector $\mathbf{n}_t$ as an independent field, and deriving from additional (orientational) balance laws independent differential equations [2]. These differential equations describe the independent rotation of the rigid mesogens connected with the flexible polymer chains. The orientation-dependent stress law of LCEs arises from an anisotropic free energy, comparable with fibre-reinforced materials [3]. But, in contrast to [3], the direction vector of an LCE model has to be independent.
In contrast to [2], we apply a variational principle for deriving a new mixed finite element (FE) formulation, which is based on drilling degrees of freedom for describing the mesogens rotation [4]. This principle leads to an extended set of balance laws which is preserved by an energy-momentum scheme.

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A Simple Fully Nonlinear Triangular Shell Finite Element

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Key Words: *Triangular Shell Element, Nonlinear Shell Formulation, Finite Rotations, Large Strains.*

Shells are one of the most important models in solid mechanics since many structures in engineering may be associated with it: metal sheets-based products, slabs, thin-walled pressure vessels, and other objects with one of its dimensions considerably smaller than others. Shell models may be adaptable to finite element usage, but some particularities must be watched it, such as locking behaviours.

This work aims to study and develop a nonlinear formulation for shells models using a special simple triangular shell element, which is a new displacement-based triangular shell element with 6 nodes. Moreover, the shear locking and membrane locking behaviour are not observed at the performance of this new element.

In formulation of shell models, we consider finite strains, large displacements, and rotations. Rotation field is re-parameterized in terms of the Rodrigues rotation vector, resulting in a simpler update of rotational variables. The Reissner-Mindlin kinematical assumption and an initial plane reference configuration for the shell is considered here.

A computational implementation is done with several numerical examples using the new element developed here. Furthermore, a comparison with numerical examples using the well-known element T6-3i [1], a six parameter (3 displacements and 3 rotations) element, is done with the aim to also illustrate the robustness of our formulation.

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An objective and path independent geometrically non-linear ReissnerMindlin shell formulation

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Key Words: shell analysis, large rotations, objectivity, path independence, manifolds, isogeometric analysis, geometric finite elements

Development of geometrically exact, non-linear shell formulations for large rotations has been subject to intensive research for several decades. A lot of progress has been made and many issues are well understood today, but there are also still some open questions. Many existing formulations suffer from singularities due to the non-linear space of the unit sphere. Additionally, some of the existing models proved to be non-objective and exhibit artificial path-dependency. For one-dimensional spatial rod finite elements these problems have been solved by Crisfield and Jelenić [1]. For shell models with Reissner-Mindlin kinematics, however, they seem to persist. We present an efficient, robust, objective, singularity-free and path independent geometrically non-linear Reissner-Mindlin shell formulation for arbitrary ansatz spaces. In particular, this formulation utilizes the ideas on geometric finite elements presented by [2] and [3] for the interpolation on non-linear manifolds. Additionally, we compare three different interpolation schemes that can be found in literature, where two of them are applied for the first time to Reissner-Mindlin shells. Path independency and objectivity of the formulation are verified via a set of numerical examples.

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Experimental investigation and mechanical characterisation of cables

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Key Words: *Orthotropic Material, Pure Bending, Reproducibility, Internal Structure*

Cables are long and thin structures that are used not only for electrical but also for structural purposes. With the increasing demand for electro-mobility and with the advances made for industry 4.0, the use of cables in cars, robots, and various other areas has increased in recent times. For such applications, they should be able to sustain the loads applied on them for a certain period of time. This leads to complex cable constructions with various layers of different materials across the cross section. The layers consist of metallic wires, dielectric layers, conducting sheaths, polymer insulations, among other types of materials.

The complex structure and construction lead to anisotropic material behaviour, where the tensile stiffness is much higher than the torsional and bending stiffness. The inner structure of the cable contributes to the coupling of the stiffnesses in all three directions of tensile, torsional, and bending loads. With the application of the bending or torsional loads, the metallic wires can move against each other, which leads to the production of tensile forces. Thus, to determine the behaviour of the cable the coupling of the stiffnesses should be considered during experimental characterisation.

To this end, an experimental setup has been constructed to test the cables under tensile, pure bending and pure torsional tests. To compensate for the tensile forces occurring during the bending and torsion experiments, the two ends of the cable are moved during the load application with the help of linear motors along its axis. The three types of tests were used for characterising a single core and a coaxial cable. Furthermore, coupled loading was also applied to see the effect of pre-torsion on the bending of cables. The experimental results of bending different cable samples were not always reproducible, because of the random orientation of the metallic wires. Moreover, as the cables are cut from different areas of a spool, the already existing curvature also varies from sample to sample. Therefore, an initial loading was applied to condition the samples, which led to an increase in reproducibility. An anisotropic elasto-plastic material model was implemented using the finite element method to simulate the behaviour of cables [1]. The discretisation of the long and thin structure was achieved with high order 3D hexahedral elements. Parameters for the model were identified with the help of tensile and torsion tests and were validated with the bending experiments. Thus, a complete experimental characterisation of cables and its simulation is presented.

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Intrinsically selective mass scaling for hierarchic beam, plate and shell formulations

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Key Words: *Selective Mass Scaling, Hierarchic Formulations, IGA.*

Hierarchic shear deformable Reissner-Mindlin shell formulations possess the advantage of being intrinsically free from transverse shear locking through reparametrization of the kinematic variables, see for instance [1], [2], among others. This reparametrization yields beam, plate and shell formulations with distinct transverse shear degrees of freedom.

The efficiency of explicit dynamic analyses of thin-walled structures is limited by the critical time step size, which depends on the highest frequency of the discretized system. In case of discretizing a thin structure with Reissner-Mindlin type shell elements, the highest transverse shear frequencies limit the critical time step, while being of minor importance for the structural response. Selective mass scaling aims at scaling down the highest frequencies, while ideally keeping the low frequencies unaffected. In most concepts, this comes at the cost of non-diagonal mass matrices. Selective mass scaling was initially invented for thin solid and solid-shell elements, but the extension to the rotational part of standard shell elements is not straightforward. Thus, mostly conventional mass scaling of the rotational inertia is used in commercial explicit codes, as can be seen for instance in [3] in the context of isogeometric shell analysis in LS-DYNA.

In this contribution, we present recent investigations on selective mass scaling with hierarchic isogeometric structural element formulations. Since hierarchic formulations possess distinct transverse shear degrees of freedom, they offer the intrinsic ability for selective mass scaling of the shear frequencies, while keeping the bending dominated frequencies mostly unaffected and retaining the diagonal structure of a lumped mass matrix. We discuss the effects of transverse shear parametrization, locking and mass lumping on the accuracy of results and a feasible time step.

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Modelling Collisions and Fluid-Structure Interaction for Highly Flexible Cosserat Rods

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Key Words: Fluid-Structure Interaction, Cosserat Rods, Collision Modeling

Aquatic canopies formed by flexible submerged plants are an essential element in river hydraulics through the flow resistance they provide, their resilience against bed erosion, etc. Knowledge about these processes is usually drawn from experiments. Only recently simulations with deforming blades have been conducted, still with relatively rigid blades [1]. In the present contribution a numerical method is presented which extends the one of [2], [3] towards long, highly flexible blades as they reconfigure, collide, and interact with the surrounding flow. It is composed of the following elements: a Navier-Stokes solver for incompressible flows with Large Eddy subgrid-scale modelling, an Immersed-Boundary-Method (IBM) for coupling, and a Finite-Difference solver according to [4] for geometrically exact Cosserat rods. The IBM is particular in that it incorporates the fluid-structure coupling by a semi-implicit approach, thus yielding very good stability, even with vanishing thickness as well as small or even vanishing mass of the blades. Another challenge arises from the structure-structure coupling via contact and collision. It is treated with a constraint-based method and turned out to provide difficulties of appropriately discretizing these constraints. To cope with these, a number of enhancements over [3] had to be developed. The capabilities of the resulting method are illustrated with first results from a large-scale simulation of 528 flexible blades in a turbulent channel.

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New Experimental Characterisation of Cable Systems

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Key Words: *Cable Bundle, Material Characterisation, Coupled Loading*

Large capital-investments are being made on cable systems especially in the automotive field. Due to the strong growth in the digitalisation of vehicles, a considerable increase in the number of cables can be seen in them. Cable bundles and harnesses are used for better cable management in these vehicles. Each cable bundle is made up of various cables and each of these cables are complex components consisting of a multi-layer structure made up of various materials. In order to characterise these cable bundles, the prediction of the effective mechanical properties of the system as a whole is focussed on.

Due to their construction, the interaction between the different components in a cable bundle leads to deviation from classical material behaviour [1]. The bending movement induces friction between the cables resulting in non-linearity effects as well as coupling between the bending and torsion load cases [2]. These non-linearity effects are analysed on the basis of the data obtained from the experiments.

For this purpose, a new test rig has been designed and built, allowing the implementation of the decoupled load cases: bending, torsion and uniaxial tension, as well as their superposition on the slender flexible structures. In particular, it is possible to investigate the highly complex effects resulting from the different structure of the various cable systems, which are directly reflected in the different behaviour of the individual systems. Three types of tests are performed, nonlinear pure bending, nonlinear torsion, and bending coupled with torsion. A large number of experiments on different cable systems with a sufficiently high number of samples were performed and the elasto-plastic behaviour of higher bending moments was compared to pure bending. A neural network for modelling cable systems was developed, which is trained with the data from experiments.

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Viscoelastic Glass Plates Co-Sagging Simulation Coupled with Air Suction

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Key Words: *Fluid-structure interaction, viscoelasticity, glass sagging, air suction*

An axisymmetric fluid-structure interaction (FSI) model, for simulating the circular glass plates viscoelastic co-sagging process with air suction, is developed in the commercial software COMSOL. The two glass plates are modelled as viscoelastic structures which are sagging under gravity at elevated temperatures with their viscosity dependent on the temperature. Generalized Maxwell model of stress relaxation is implemented for simulating the viscoelastic behaviours. The air suction is implemented with a thin film flow based on the Reynolds equation of the lubrication theory. Numerical case studies are performed to understand the fundamentals of the two glass plates interaction with the air film layer and impact of process parameters.

It is discovered that the air suction pressure increases when the viscosity difference between the top and bottom glass plates becomes larger. When the viscosities are the same, the pressure is close to zero. The pressure increases with the top-bottom glass viscosity ratio and reaches a peak value when the viscosity ratio is above 1000. The peak value is equal to the weight of the bottom glass.

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Discrete Network Models inspire a new class of Continuum Constitutive Models for Fibre Network Materials

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Key Words: Fibre Networks, Multi-Scale Modelling, Homogenisation, Constitutive Modelling

Multi-scale mechanical models allow to infer microscopic information from the macroscopic response. Two-scale models of fibre network materials are relevant in many fields of engineering, but also in computational mechanobiology problems, where tissue-scale loads are transfered to the cell scale through a collagenous network to provide the cues for various cellular processes [1]. Discrete network models (DNMs) are a common strategy for two-scale problems. DNMs reveal micro-scale information far beyond real experiments and challenge the macro-micro transitions used by the majority of the common continuum mechanical concepts, but also provide the basis to develop novel approaches.

One piece of information is the distribution of fibre stretch within the network [1, 2, 3]. Based on studying various DNM representative volume elements (RVEs) of generally non-linear elastic fibres, we propose a constitutive relation between this micro-kinematic distribution and the macroscopic deformation imposed via the boundary conditions. Our analysis revealed a strong resemblance of the obtained stretch histograms with the log-normal distribution $\mathcal{L}$. Describing $\mathcal{L}$ in terms of the macroscopic deformation, this novel approach yields excellent agreement with the homogenised stress and energetic response of the DNM RVE, and at the same time preserves the micro-kinematic information on the distribution of stretch, making it a promising tool for efficient computational analysis of fibre network materials.

Finally, we discuss methods to overcome the costly generation of a numerical DNM ground truth needed to parametrise the model, and sketch strategies to obtain the relevant information for model calibration from real experiments.

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Modal tests of inflatable wings based on distributed MFC actuators

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Key Words: *Inflatable Wings, Dynamic Characteristics, MFC Actuator, Wet Mode*

Inflatable wing is a multi-cavity inflatable structure made of high-strength composite flexible material and filled with high-pressure gas to maintain airfoil. Due to advantages in light weight, convenient collection, rapid expansion and low cost, inflatable wings provide a more flexible technical solution for aircrafts with limited space to launch, such as small and medium-sized UVAs, cruise missiles and gun-launched missiles. The structural dynamic characteristics of inflatable wings are complicated because of the high flexibility and light weight, and traditional methods for rigid wings are no longer applicable. In modal tests for inflatable structures, especially for complex structures with high flexibility like inflatable wings, traditional modal testing technique using hammer or shaker is questionable to excite the global modes of the structure without local overexcitation. The variety of sizes, low mass, and fast time response of the Macro Fiber Composite (MFC) make it an excellent candidate for use in the dynamics and control of inflatable structures. In this paper, a distributed excitation system is proposed based on MFC actuators for modal tests of a flexible lightweight inflatable wing, and the dynamic characteristics of the inflatable wing are analyzed. Firstly, a finite element modelling and modal analysis of an inflatable wing is carried out. Since the inflatable membrane with high flexibility is barely able to endure out-of-plane load, which converts the load into in-plane tension in the form of membrane prestress. And the contribution of added air-mass to the vibration system cannot be ignored. Wet mode considering membrane vibration theory and added air-mass is applied to obtain modal parameters and provide reference for modal tests. Then, a distributed excitation system based on MFC is set up, and an example of simple supported beam is given to verify the feasibility of system. Finally, dynamic characteristics of inflatable wings is analyzed based on MFC excitation system, and the type, number and distribution of MFC are designed to improve the experiment performance. The results show that the distributed excitation system based on MFC is capable to excite global mode of inflatable wings. Besides the spanwise bending and torsional mode, inflatable wings also present chordwise bending mode, which is markedly distinguished from the traditional rigid wings.

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A mixed finite-element formulation for axially moving continua

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Key Words: Axially moving continua, mixed finite elements

We present a novel approach for the analysis of axially moving continua, i.e., structures that are characterized by a translational motion in one of their preferred directions. Axially moving continua occur in many important industrial processes as, e.g., rolling mills, in which material is (more or less) continuously transported through the plant. Challenges in modeling and simulation of axially moving continua are manifold: First and foremost, the underlying translational motion is adverse to a Lagrangian formulation of continuum mechanics, in which physical fields are related to material points of the structure. Diverse variants of *Arbitrary Lagrangian-Eulerian* (ALE) and *mixed Eulerian-Lagrangian formulations* have been proposed to account for the fact that material points located in the domain of interest vary due to the translational motion. Secondly, we typically deal with thin-walled structures that are subjected to large deformations. For this reason, structural theories for beams and shells are often adopted in the computational analysis. On top of that, the material behavior is inelastic in many industrial processes. Non-Lagrangian formulations therefore require transport schemes for internal variables that govern the stress response and constitutive relations need to be translated to structural theories.

We address the challenges of axially moving continua by combining an effective mixed finite-element formulation for three-dimensional continua with a generalization of the *sliding-beam formulation* [1], i.e., a non-material description for sliding structures and axially moving continua. In particular, we use the *tangential-displacement normal-normal-stress* (TDNNS) method by Pechstein and Schöberl [2]. The TDNNS method is based on the idea of relaxed continuity in displacement and stress fields across element faces. TDNNS elements have proven superior performance in problems of thin-walled structures as compared to conventional irreducible formulations, since they do not suffer from shear locking. We apply the coordinate transformation of the sliding beam formulation to the three-dimensional relations of continuum mechanics, on which the TDNNS formulation is based. The proposed approach allows us to effectively analyze complex problems of axially moving continua without resorting to structural theories.

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Geometrically Exact Dynamics of Sliding and Rotating Nested Rods for Modeling Concentric Tubes Robots

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Key Words: Sliding rods, Geometrically-exact methods, Continuum robotics

Continuum robot architectures find wide application in medicine since they can be designed to achieve a high ratio of length to width, making them well suited to minimally invasive interventions. These designs are distinguished by using deformable elongate elements whose shape, theoretically, requires an infinite number of degrees of freedom to model. Concentric Tube Robots (CTRs), a collection of nested millimeters tubes, belong to this category. A general architecture comprises three tubes: a fixed, relatively rigid, straight tube that serves as a guide and two flexible concentric tubes with a pre-designed 3D curved shape. CTRs can be controlled through its proximal end, outside of the patient. The physician regulates the relative sliding and rolling of the tubes, whose elastic interaction determines the overall shape of the system and the iteration force at the end-effector for surgical intervention. The accurate control of the CTR navigation and tissue interaction requires the development of sophisticated mathematical models. Although significant results have been achieved, only quasi-static motion of the tubes' sliding has been considered so far [1].
Here we present a complete dynamic model of the three tubes architecture described above, including the sliding phenomena. To do so, a Cosserat model of the rods' deformation is employed, parametrized using a novel, geometrically-exact, Ritz-like reduction of the beam's strains [2]. In the context of CTRs, it allows selecting the active strains of a general Simo-Reissner beam that satisfy the distributed constraints imposed by the rods' concentricity, eliminating from the equations the complex inter-tubes constraints force. Due to the tubes' sliding, the domain of the overlapping sections comprising the CTRs "grows" or "shrinks" as a function of the insertion parameters. Once this additional motion is included in the geometrically-exact kinematics of the Cosserat rod, the d'Alembert's principle can be applied to obtain the equations of motion in the usual Lagrangian form, suitable for control. In the static setting, this procedure allowed calculating the insertion forces required for the equilibrium for the first time [3].

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Mixed Eulerian Lagrangian approach in Rolling Mill Simulations

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Key Words: Finite Element Analysis, Mixed Eulerian Lagrangian Description, Material Generation

We present a mixed Eulerian-Lagrangean approach used for simulating the strip run in rolling mills. The simulation tool is intended to be finally used for optimizing parameters of attached software controllers before they are implemented at the real plant, an intention which imposes two more or less contrary requirements concerning the final product: On the one hand it should be highly accurate to allow finding near optimal and reliable controller settings for real life application. On the other hand – since a large number of single simulations will have to be run in order to find optima in a multidimensional parameter space – it should be particularly fast. A standard type approach (such as using standard 3D Finite Elements undergoing 3D contact analysis at the roll gap) would miss to exploit specific problem characteristics and thereby be lacking performance.

A more modular approach is presented, which is particularly adapted to the underlying problem and has evolved throughout the last decade of co-operation between Primetals Technologies Germany, Johannes Kepler University Linz, and Linz Center of Mechatronics GmbH on this topic.

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Non-material kinematic modelling in roll forming of steel sections

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Key Words: roll forming, mixed kinematic modelling, axially moving continua, finite element analysis

Roll forming is a manufacturing process which is classified among the cold forming processes [1]. Here, an initially flat metal sheet is continuously fed through several forming passes. Each forming pass consists of a pair of contoured rolls which contribute incrementally to the total bending deformation. The final cross section shape is obtained by irreversible plastic bending deformation, membrane strains remain small. Furthermore, no significant deformations in thickness direction occur during this process.

Lagrangian finite element formulations are traditional in structural mechanics. This becomes, however, inefficient for axially moving continua, as material particles keep entering and leaving the control domain, as it is the case in roll forming. Numerically induced oscillations are inevitable because of the spatially localized contact forces acting at moving finite elements. Moreover, no mesh refinement near the contact locations is possible. Using the mixed Eulerian-Lagrangian description, we restrict the attention to the active domain of interest. The issues regarding the numerical oscillations and mesh refinement are no longer relevant, as material particles flow across the mesh. For this sake the nonlinear structural equations need to be transformed to a different set of coordinates, namely an Eulerian one in the direction of the movement and Lagrangian coordinates for the transverse and out-of-plane directions [2, 3].

For an alternative attempt to treat the roll forming process using ALE kinematic formulation with the help of the non-material 3D continuum elements we refer to [1]. In the present contribution, we make use of the shell model of the metal sheet, which shall be computationally more efficient. Moreover, the plastic deformations are treated both, on the level of continuum mechanics featuring an integration over the through-the-thickness element of the shell as well as on the structural mechanics level, which is based upon a novel problem-oriented plasticity model for a shell [4].

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Sticking and sliding of an endless elastic strip on a moving rough surface

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Key Words: axially moving continua, non-material finite element analysis, frictional transport

Axially moving deformable structures play a central role in various technical solutions like belt drives, rolling mills, winding of coils, etc. Inertia and elasticity of the moving structure, geometric and material nonlinearities as well as contact phenomena altogether result into non-trivial and sometimes counter-intuitive response of such structures to geometric imperfections or external actions. Nowadays, growing attention is paid to dynamical systems, in which the time evolution of the deformed state of an axially moving structure is possible even quasi-statically at slow motion because of nonlinear contact interactions. Examples are the elastic-plastic bending of a metal strip in a roll forming machine [1], motion of sheet metal between the roll stands of a hot rolling mill [2] or the elastic deformation of a steel belt owing to the dry friction in the moving contact pairs of a steel belt drive [3].

The last example of a frictional transport problem motivates the study of the motion of an elastic strip travelling on a horizontally moving rough plane. The lateral misalignment of the guideways at the entry to the control domain and at the exit from it enforces the deformation of the strip and makes sliding inevitable, at least in the part of the domain. An analytical quasi-stationary solution featuring infinitely many self-similar segments of sliding followed by a zone of sticking contact was obtained under the assumption of Bernoulli-Euler beam model of the strip in [4]. In the present contribution we release some of assumptions of the analytical study and consider refined models of the moving strip: the Timoshenko beam model and the two-dimensional plane stress formulation. The mixed Eulerian-Lagrangian kinematic description implemented in form of non-material finite element formulations allows both the transient and the quasi-stationary analysis of the axially moving elastic structure with friction.

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Out of Plane Lower Bound Limit Analysis

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Key Words: *Masonry plates, Failure analysis, Lower Bound Limit Analysis, Linear Programming problem, Homogenization approach.*

Surveys conducted after severe seismic sequences all around the world and fragility curves produced with techniques at territorial level, plus experimental tests show that the most diffused collapses occurring for existing masonry buildings are partial out-of-plane failures of large rigid portions with variable shape, roto-translating and forming a pre-defined kinematic chain, whose shape depends on several concurring factors, such as masonry texture, membrane loads and the interlocking between perpendicular walls.

Compared with the in-plane studies, the experimental research on out-of-plane loaded masonry is less abundant. Limit analysis seems the most suited tool to deal with the determination of the behavior at failure of out-of-plane loaded masonry panels.

A novel Lower Bound Limit Analysis Finite Element model for the study at failure of masonry walls in two-way bending is presented. In the model, a masonry plate is discretized into infinitely resistant hexahedrons and quadrilateral interfaces where all plastic dissipation occurs. Three internal static variables act on interfaces, namely bending moment, out-of-plane Kirchhoff shear and torque. Equilibrium is imposed on hexahedrons, whereas admissibility is enforced exclusively on interfaces between adjoining elements. The admissibility of the internal actions on masonry interfaces is imposed with a strength domain obtained by means of an already existing LB homogenization technique where joints are reduced to interfaces. The resultant Linear Programming (LP) problem - which allows to estimate collapse loads and distribution of internal actions at collapse - is characterized by a number of variables and constraints relatively limited, which requires a very limited computational burden to be solved through standard interior point LP software. Failure mechanisms are obtained solving the dual LP problem.

The procedure proposed is validated against two existing experimental data sets, namely three series of walls with slender perpendicular walls connected on vertical edges and tested at the University of Adelaide (Australia) [1] and four series of solid (one) and perforated (three) panels tested at the University of Plymouth (UK) [2][3]. A high accuracy of the model proposed in the prediction of the load carrying capacity, failure mechanism and distribution of internal actions at collapse has been found.

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Seismic Vulnerability Assessment of Historic Masonry Buildings through Fragility Curves Approach

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Key Words: *Historical Heritage, Seismic Vulnerability Assessment, Fragility Curves Application,*

The assessment of the seismic vulnerability of built heritage is still an open issue. Regarding this topic, in recent years many researchers have worked in the development of refined numerical models to simulate the behaviour of different building typologies subjected to seismic action. To be reliable, these models require in-depth knowledge of the building object of study.

In many countries, such as Italy, where the widespread historical heritage is widely present, there is the need to define quick, but reliable, evaluation procedures, which allow, in advance, to assess the vulnerability of the historical heritage of an entire area using databases already present without necessarily proceeding with detailed investigations on each building. This procedure has already been adopted in some case studies to compute a vulnerability index [1] or a safety factor for the structures examined [2].

Based on procedures in the literature, the authors have developed a forecasting methodology focused on the construction of fragility curves, safety factor vs PGA and vulnerability index, which allows to formulate hypotheses on the probable behavior of a specific type of building, to any similar actions and the probable expected damage. In the view of proceeding to the safety of a small historic village in an area with a high seismic propensity, this procedure could be useful for prioritizing interventions in probabilistic terms.

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The non-smooth tale of Accumoli civic tower

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Key Words: *Masonry, Non-smooth contact dynamics, Distinct Element Method, Concrete Damage Plasticity*

The dynamics of historical masonry buildings is one of the most difficult tasks to be investigated in structural engineering, since these kinds of structures are commonly heterogeneous, with complex geometry, and with unknown quality of the connections between different structural parts, in particular walls and floors, that often play a crucial role. However, understanding the dynamical behaviour is crucial for a reliable seismic vulnerability assessment, which became more and more important due to recent catastrophic earthquakes (Umbria-Marche 1997–1998, Abruzzo 2009, Emilia-Romagna 2012, Marche-Lazio-Umbria-Abruzzo 2016).
In this work, the nonlinear dynamics of a medieval tower located in Accumoli, a village in central Italy, recently damaged by earthquakes is investigated. Generally, the mechanical response of masonry towers is commonly investigated by finite element methods [1], often including very sophisticated constitutive laws considering post-elastic behaviours and damage. These methods, while being very appealing, do not focus on the possible non-smooth nature of the dynamic response, which can come sliding and impacting between different blocks, and situation that is common just before and during the collapse. For this reason, in the present paper, the dynamics of the tower, schematized as a set of rigid blocks, is investigated by means of a distinct element code that implements the Non-Smooth Contact Dynamics method (NSCD) [2].
The main goal is to determine the weakness zones of the structure during seismic events, and the possible collapse mechanisms.
Harmonic oscillations applied to the basement of the tower are considered first, and a systematic parametric study is done, aimed at correlating the tower vulnerability to the amplitude and frequency of the excitation. In addition, numerical analyses are performed to see the effects of the friction coefficient and of the block's geometry on the dynamics, and on the collapse modes.
Then, the study of the tower stability against recorded seismic excitations is addressed. Attention is paid to the occurrence of out-of-plane torsional overturning mechanisms, and some comparisons of the damage obtained with the present approach and with other numerical models, like continuous finite element approach, are reported.

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Unbonded Fiber Reinforced Elastomeric Isolators (UFREIs) made of high damping natural rubber blends

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Key Words: *Seismic isolation, Unbonded fiber reinforced elastomeric isolator (UFREI), High Damping Rubber, Finite Element analysis, nonlinear dynamic analysis.*

In the last four decades, some commercial base isolators have been introduced to protect buildings from vibration and earthquakes. Typically, they are constituted by several alternating layers of rubber pads and steel interposed by two continuous pads, having the role of limiting vertical deformability. At the same time, they exhibit good deformation capacity in the horizontal direction when subjected to a seismic load. A very effective seismic isolator shall satisfy the following functions: good performance under all service loads, vertical and horizontal; provide enough horizontal flexibility to reach the target natural period for the isolated structure; recentering capability after the ground motion, so that no residual horizontal displacement can downgrade the serviceability of the structure; provide an adequate level of energy dissipation (damping) to control the displacement that could damage other structural members. Steel-reinforced elastomeric isolators (SREIs) is the most used method of seismic isolation. Since these devices are generally too expensive due to the need to introduce thick steel plates for their supports and the high energy consumed for the manufacturing process, they are not suitable for ordinary residential buildings, especially in developing countries. Compared with SREIs, fiber-reinforced elastomeric isolators (FREIs) have considerably lower weight and can be manufactured through cold vulcanization [1][2]. They could be installed between the structure in elevation and the foundation without any bonding or fastening in the so called unbonded application (UFREI), reducing costs hugely [3][4][5][6]. Furthermore, without steel supports, the shear load is transferred through the friction generated between the isolator and the structure surfaces, improving the dissipation energy of the devices. The main feature of such a UFREIs is the large deformability thanks to the roll-over deformation and the favorably lower lateral stiffness compared to the bonded isolator [7]. In this paper, a series of experimental tests and numerical analyses have been performed to investigate the seismic behavior of UFREIs made of high damping rubbers (HDR) combined with glass fiber reinforcement. In particular, two HDR have been considered. The first one consists of a Natural Rubber and Bromobutyl (NR-BIIR) blend. Instead, the second one is constituted of a NR and Ethylene Propylene Diene Monomer (NR-EPDM) blend. Results obtained from FE cyclic shear tests analysis and nonlinear time history analyses of structural application have shown that the devices are suitable to isolate low-rise masonry buildings properly.

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Actuation of concrete slabs under bending with integrated fluidic actuators

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Key Words: *adaptive structures, slabs, integrated actuators, Multi-axial load transfer*

In previous researches it has been shown that 33 % to 44 % of the mass in residential and office buildings and up to 50 % in high-rise buildings is attributable to floor slabs [1, 2]. Floor slabs typically take loading through bending. Such a load-transfer mechanism is not efficient, since the material in the proximity of the neutral plane is practically unloaded thus resulting in a poor utilization rate. Since bending stiffness is significantly lower than axial stiffness in a slab, typically deflection limits under out-of-plane loading govern the design of floor slabs. This causes significant oversizing. In addition, structures are typically oversized since they are designed to take extreme loading events, which in practice occur only for a small part of the service time. The on-going climate crisis, the expected world population growth and associated resource scarcity, call for new methods and solutions to build material-efficient structures with low embedded greenhouse gas emissions [3]. Employing adaptive structures could provide solutions. By integrating structures with components such as sensors, actuators and control units – stress and deformation caused by changing loads can be reduced actively, which enables significant material savings [4, 5]. Previous work carried out at the University of Stuttgart within the Collaborative Research Center 1244 has demonstrated that it is possible to compensate deflections by integrating fluidic actuators in beam structures subjected to bending [6]. However, it is not obvious how to transfer actuation strategies employed in beams to floor slabs due to multi-axial behaviour. In this work fluidic actuators are strategically integrated into floor slabs to employ multi-axial force transfer to counteract the effect of out-of-plane loading. The research also addresses the choice of an optimal distribution and layout of the actuators. Numerical simulations of different actuation strategies, such as uniaxial and biaxial actuation have been carried to derive influence fields. The relationship between principal moments and the influence of actuation is quantified numerically. Examples are provided to show how influence fields can be employed to select suitable actuation strategies. Results show that displacements can be efficiently compensated through a combination of uniaxial and biaxial actuation.

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Control Strategies for Adaptive High-Rise Structures

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Key Words: Building automation; optimal control; adaptive structures

The growing world population and the increasing urbanization worldwide leads to continuous growth in the global construction activity. The building sector is responsible for about 35% of global green house gas emissions and more than 50% of resource consumption. Therefore, integrating innovative technologies into buildings is an important step towards achieving the climate and environmental policy goals, such as the Paris climate protection agreement.

The concept of adaptivity offers a way of reducing the material consumption by half. However, the mass reduction leads to multiple challenges such as increased susceptibility to static loads, e.g. snow, and oscillations resulting from dynamic disturbances as wind and earthquakes [1]. Adaptive buildings comprise sensors, control units and actuators and are able to actively counteract external disturbances. Furthermore, the active control strategy needs to take into account component failure in order to maintain the high safety standards of the construction sector.

The world's first adaptive high-rise building is built at the University of Stuttgart, Germany. The state of the building is measured by strain gauges and an optical measurement system, identifying the nodal displacement. Hydraulic cylinders, integrated into the structural elements, are able to actuate the structure in order to counteract static and dynamic disturbances.

A control law for compensation of static loads under consideration of the limited actuator forces is presented in [2] and validated using simulations and a scale model of the adaptive high-rise structure. Furthermore, our research group developed multiple control strategies for vibration damping, including linear quadratic controllers [3, 4, 5] and a model predictive controller. Experimental validation of the proposed control approaches is important but yet to be done. In this work, we will present some early validation results.

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Effective range of integrated fluidic actuators in structural elements

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Key Words: *adaptivity, lightweight construction, beams, slabs, integrated actuators, simulation*

A high demand for living and working space as well as the corresponding infrastructure, caused by a growing population and increasing prosperity worldwide, leads to an increased consumption of mineral resources. This is accompanied by a high usage of grey energy and a high output of greenhouse gas emissions. For example, the cement production is responsible for up to 10 % of global anthropogenic CO_2 emissions [1]. In addition, the design of conventional building structures must be based on relatively high loads or load combinations that rarely or even never occur. Thus, today's conventional structures are oversized for most of their lifetime.
Adaptive structures represent a promising approach for mass and resource savings. Through the interaction of actuators, sensors and control units, the structure can adapt to the external loads to reduce stresses and deformations. As a result, material input can be reduced. [2]
In order to respond to all possible load cases, the structural element has to be manipulated locally. For structural elements subjected to bending loads, it is advantageous to integrate actuators into their cross-section to optimize the load transfer and thus achieve material savings. Fluidic actuators are a suitable solution due to their high energy density. However, they must be designed for this application. This is part of the subproject ‘C02’ of the Collaborative Research Centre 1244. The functional capability has been demonstrated for beams made of concrete in various simulations and on functional samples [3]. Therefore, actuators were integrated into the compressive zone of the beam. By applying forces in the longitudinal direction of the beam, a moment is generated that counteracts the bending moment caused by the external load. The effective range of the generated moment is limited, since the force is directly short-circuited via the concrete surrounding the actuator. For actuators in slabs, new challenges arise due to the multi-axial load transfer. In particular, the aim is to achieve the largest possible effective range of the applied moment in order to reduce the number of integrated actuators required. One approach is to optimize the geometry of the force-introducing surfaces inside the structural element.
This contribution presents a study about the correlations of the geometric parameters. Here, numerical simulations are used to determine these correlations. Based on the results, an analytical approach is formulated that describes the impact and area of influence of the intra-structural force application. Thus, the geometric and mechanical interface between the structural element and the integrated actuator can be pre-dimensioned. A first step towards the design of an adaptive element with integrated actuators subjected to bending is hereby possible.

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Fault Diagnosis for Adaptive Structures

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Key Words: fault diagnosis, adaptive structures

Adaptive buildings can dynamically adapt to changing external loads using integrated actuators, and thereby significantly reduce the resource consumption and the emissions in the course of the building's construction [1]. Given the large number of sensors and actuators in such an adaptive building, in combination with its long lifetime, failure of one or more of those components is likely. This is generally referred to as a fault, and comprises different types of failures ranging from a bias in a sensor's measurements or the force provided by an actuator, to the total unresponsiveness of the component. As adaptive buildings are operated in a closed control loop, such faults directly affect the control inputs, i.e. the forces applied to the building by the actuators, and can thereby compromise the building's functionality and safety. A reliable fault diagnosis system that detects and classifies faults promptly and reliably is a prerequisite for initiating suitable countermeasures in case of a fault, and is therefore essential for any adaptive building.

For both purely model-based and hybrid model-/data-based approaches, simulation studies considering an adaptive high-rise building revealed a detection and classification of such faults with high accuracy [2], [3]. Lacking a suitable experimental platform, however, these methods could not be validated on a real-world adaptive structure until now.
Using a recently constructed demonstrator building, an adaptive high-rise truss structure of 36 meters in height located on the campus of the University of Stuttgart, we now provide such an experimental validation. In order to successfully transfer the methods for fault diagnosis from simulation to a real-world setting, model errors are a major challenge and can cause a significant drop in performance. Previous simulation studies did not consider model errors exceeding simple parametric errors in a linear state space model, which are not representative for the model errors encountered in real-world conditions. In that context, we investigate the suitability of different methods for fault diagnosis by evaluating their performance in a real-world setting.

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Formulation of actuation units for stress-free control of deformations in statically indeterminate adaptive structures using actuation influence matrices

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Key Words: *Adaptive structures, influence matrices, actuation units, stress-free*

The construction sector contributes considerably to material resource depletion and it is responsible for a large share of global emissions. Given the growing world population and related demand for new built environments, new approaches are needed to significantly reduce the environmental impact of the construction sector. One proposed solution are adaptive load-bearing structures [1,2]. Actuators, sensors and control units are strategically integrated to manipulate deflections and stress under loading, which results in significant material and emission savings. Current research is looking into actuation strategies, optimal actuator placements as well as structural topologies that result in material- and emission-efficient adaptive structures. A useful method for analysing the capabilities of adaptation of spatial trusses and frames are actuation influence matrices [3]. These matrices contain quantitative information on how nodal deformations, normal and shear forces or bending moments can be influenced through actuation for a given structural topology – independently from a specific control objective (inherent adaptivity). A row gives the influence of actuation of each element on the selected structural response e.g., the corresponding displacement or element force. A column gives the influence of actuation of the corresponding element on the structural state e.g. the state of normal forces or nodal deformations. The rank of an actuation influence matrix is thus equal to the number of linearly independent states that can be induced through actuation. Forces, moments and displacements resulting from actuation can be computed by multiplying the individual columns with an actuation input load.

Combining multiple columns of an actuation influence matrix allows for the formulation of so called actuation units [4]. These actuation units can be employed to model physical actuators spanning over multiple elements or to predefine a specific relation in which multiple elements are to be actuated (constraint equation). For example, to guarantee stress-free control of deformations in statically indeterminate structures. A method is derived to formulate actuation units for stress-free deformation control showing that its general applicability can be assessed from the rank of the actuation influence matrices.

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Optimization-Based Studies on the Integration of Load Alleviating Deformation Behaviour in Active Morphing Wing Sections

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Key Words: *Morphing wing, adaptive structure, load alleviation, multidisciplinary optimization*

Morphing wings are currently of high research interest in the field of adaptive structures. They promise to increase the efficiency and mission adaptability of future aircraft. By replacing discrete high-lift and control surfaces, the aerodynamic efficiency can be improved. Furthermore, by adapting the wing to its optimal shape for each flight condition, fuel consumption over the whole flight mission can be reduced. Despite the promising benefits of morphing wings, significant increases of the wing mass have to be expected. Moreover, the energy required for active shape deformation reduces the net reduction of fuel needed. Therefore, lightweight design of morphing aircraft wings becomes even more important than for conventional wings. On the other hand, morphing wings themselves offer potential for weight reduction if they are used for load alleviation. In consequence, design loads can potentially be decreased, resulting in reduced structural masses. This motivates the necessity of enhancing active morphing wings with load alleviation potentials.

In order to obtain preliminary design suggestions for morphing wings, the multidisciplinary characteristics, arising from the combination of structural, aerodynamic, kinematic and actuation aspects, have to be taken into account. For this purpose, the authors recently presented an optimization framework for optimizing active morphing wing sections with the aim of reduced drag over a certain flight mission and low structural mass [1]. The internal layout of the morphing wing sections is defined by a truss structure [1]. Based on the resulting design proposals for active morphing wing sections, the present work investigates the potential of combining the active morphing wing sections with a passive deformation behaviour in order to reduce loads arising from increased angles of attack, as it is typical during gust. Therefore, target-oriented stiffness reductions of individual components of the active truss structure are optimized using Evolutionary Algorithms and a loosely coupled fluid-structure interaction approach. Target is the reduction of the lift increment by passive deformation of the aerofoil section for increased angles of attack.

The optimization approach presented allows to conduct first preliminary feasibility studies that can build the basis for future morphing wing concepts combining drag reduction and load alleviation. It is shown that the investigated concept enables feasible deformations of the aerofoil contour in order to reduce undesired lift increments.

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State Estimation for Adaptive Structures

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Key Words: state estimation, adaptive structures

The construction sector causes a significant part of the global resource consumption (material, embodied energy, waste, emissions). A rising living standard and a growing world population aggravate this problem. In order to reduce the resource consumption in the construction sector, ultra-lightweight structures are helpful. Ultra-lightweight structures can be realized through the concept of adaptive structures [1]. Adaptive structures refers to structures equipped with sensors, actuators and control units. Although ultra-lightweight structures may be more susceptible to static deformation and vibration caused by loads or disturbances such as wind, snow or earth quakes. In contrast to conventional (passive) structures, adaptive structures can handle them by actively counteracting them.

For an adaptive structure to actively and effectively counteract disturbances, a control concept is required, the design of which is one of the challenges in developing adaptive structures. The main components of the control concept are a controller, a state estimator and a fault diagnosis block. The state estimator uses the sensor measurements and a dynamic model of the structure to compute the structure's state, which consists of all nodal displacements and velocities. The state is then used by the controller to compute a control signal for the actuators and by the fault diagnosis block to detect and isolate faults of sensors or actuators. Usually, the static deformation and vibration of a structure is initially caused by immeasurable, external disturbances. However, if these disturbances are unknown to the state estimator, they can lead to a significant estimation error. That motivates to develop disturbance estimation concepts, too. Within our research group, sensor placement and model-based state estimation methods have been successfully applied to and adaptive high-rise building in simulations [2, 3, 4]. In that context, we investigate simulatively methods for state and also disturbance estimation for example adaptive structures.

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Vibration control of simply supported beam bridges equipped with an underdeck adaptive tensioning system

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Key Words: *Adaptive structures, bridge engineering, vibration control*

External post-tensioning is an effective solution to improve the structural performance of beam bridges [1]. The tension force from the external cables is applied eccentrically to the neutral axis by means of deviators. The resulting system of forces induces a bending moment that counteracts the effect of the external load. However, typical external post-tensioning systems are effective under one scenario which is usually the permanent load. This work investigates the application of an external adaptive tensioning (EAT) system to the design and control of high-speed railway (HSR) bridges. The design of HSR bridges is challenging because strict criteria for safety and comfort must be met, which typically results in oversizing. Train loading can often cause a significant dynamic response. The sudden entry of a high-speed train is similar to an impact load and the excitation frequency caused by the regular spacing of the train wheels can induce resonance. The EAT system comprises under-deck cables deviated by variable-length compressive struts that act as intermediate supports. The structural system behaves as an underdeck cable-stayed bridge [2] where each cable end is fixed to the corresponding end of the beam nearby the support. However, linear actuators are employed to adjust the length of the struts, which changes the tension in the cables allowing to manipulate the bending moment as the load changes. Previous work has shown that similar external adaptive tensioning systems are effective to reduce the response of beams under quasi-static [3, 4] as well as dynamic loading [5]. A sensitivity analysis is carried out on simply supported steel-composite beam bridges to identify limitations from design best practice. Typical dimensions are considered by varying the span from 15 m to 45 m while keeping the depth to 2.4 m. Full time-history analysis shows that vertical acceleration limits cannot be met for most medium- and long-span configurations. A comparison is carried out with identical bridges equipped with an EAT system comprising a single actuator. The vertical response is reduced through the actuator length adjustments that are computed by a state-feedback controller based on the Linear Quadratic Regulator. Results show that vibration control through the EAT system enables vertical acceleration limits for medium-span HSR bridges to be met. The cyclic stress intensity range is significantly reduced demonstrating the potential for fatigue-life extension.

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An Approach for Optimal Sequential Sensor Placement Under Steady-State Dynamics

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Key Words: Structural Health Monitoring, Damage Detection, Optimal Experimental Design, Optimal Sensor Placement, Digital Twin, Structural Dynamics

Identification and monitoring of damage have a growing importance in the maintenance of structures. A robust active sensing framework that integrates model-based inference and optimal sensor placement is proposed. The approach addresses the monitoring problem with a holistic view in which inference from data and data acquisition scenarios are tightly connected. Structural health can be continuously and accurately assessed by solving an alternating sequence of damage estimation and optimal sensor placement problems.

A partial differential equation-constrained formulation for damage estimation is first developed using a conventional model-updating approach with a binary penalization damage parameter. Then, this formulation is linearized around an appropriate nominal damage state to produce an Optimal Experimental Design (OED) problem for desirable sensor locations. The sequential sensing framework is postulated using a variance-minimization approach as follows: given a current candidate damage state associated with the most up-to-date sensor information, find the next sensor location that minimizes the variance in the inferred damage state and update the damage estimator.

The sequential sensing framework is also enhanced by introducing a Modified Error in Constitutive Equations (MECE) functional in the damage estimator. Adding MECE will quasi-convexify the damage estimation problem, making the framework more robust by limiting the damage estimator from being trapped in local minima. This ensures that the sequence of damage estimation problems will converge to the true damage state given arbitrary initial guesses and sufficient sensor information.

Finally, the sequential sensing framework with MECE is demonstrated using numerical and experimental models analogous to digital twins of reactor vessel internals in nuclear power plants. Practical algorithmic heuristics including sensor placement constraints and convergence criteria are explored.

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Comparative Study of Statistical Model Calibration Framework for Li-Ion Battery Health Estimation

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Key Words: *Model Calibration, Bayesian Updating, Verification and Validation, and Li-Ion Battery*

As the commercialization of electric vehicles (EVs) progresses, high reliability of the systems in EVs like battery systems are required. For high reliability of the battery system, information about the health state of the battery system during degradation is essential. When the battery is used repeatedly, the chemical state inside the battery changes. The chemical state changes cause the degradation of battery health sates such as state of health (SOH), mechanical properties (stack pressure and swelling). Such a change in the health state is a cause of failures inside and outside the battery systems. For preventing these failures, the various studies are attempting to model and accurately predict the changes of the battery systems. There are two challenges in the predicting health state using the mathematical models. (1) Batteries of various specifications are used for each EV models, and different batteries have different parameters in the models, and (2) even within the same battery, aleatory uncertainty occurs due to chemical uncertainty. Therefore, in order to accurately predict the health state of the battery system, statistical state information in consideration of the above factors is required.

Model calibration plays an important role in the engineering field as a way to improve the results of Model & Simulation. Various model calibration methods perform the calibration process in consideration of the bias and uncertainty existing in the model or real world. The well-known KOH framework defines the model discrepancy term for the bias between the simulation model and the real data, and updates the bias through this framework. [1] And the recently studied SeCav framework is sequentially performing model calibration and validation using uncertainty quantification and reduction. [2] And the BC-TS technique performs model correction of parameters lacking prior knowledge by using the Takagi-Sugeno fuzzy models rather than the GP in the existing calibration framework. [3] This paper studies the framework of existing model calibration frameworks (1) to check whether the GP, RBF, and fuzzy models adequate for the battery bias model updating generated by different parameters for each battery, and (2) compares whether each framework statistically predicts the aleatory uncertainty of the battery system. The comparison study finds the best modelling techniques and calibration framework for the model prediction of batter systems by using the existing battery model and given data.

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DRILL STRING MODEL SELECTION AND PARAMETER ESTIMATION

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Key Words: drill string nonlinear torsional dynamics, stability analysis, bifurcation, Bayesian model selection, parameter estimation

Drill string is a slender structure that rotates to drill rocks in search of oil and gas. Its torsional non-linear dynamics is of particular interest because high oscillations might occur and should be avoided. The self excited mechanism happens due to the non-linear bit-rock interaction. There are different ways to model this interaction which lead to different bifurcation maps. We would like to stablish a methodology to choose the model that most corresponds to the available experimental data [1].

The Bayesian strategy for parameter estimation is convenient for this type of application [2]. The stochastic inverse problem begins with prior information about the probability density model of the parameters that should be identified. Then, experimental data is used to update the probabilistic model with the aid of Bayes formula, if the likelihood function is known. Statistics of the parameters and of the predictive models are obtained.

In this context, the present work proposed to apply the approximate Bayesian computation (ABC) [3], which is likelihood free, for parameter estimation, uncertain quantification and bit-rock interaction model selection. The (i) exponential, (ii) hyperbolic tangent, (iii) combined models are able to represent the non-linear interaction, but the ABC procedure indicates that the combined model yields a higher probability, considering the configuration analysed and the available experimental data.

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Learning measured bifurcation diagrams with physics-based models augmented by machine-learnt structures

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Key Words: *scientific machine learning, nonlinear dynamics, universal differential equations*

With more and more data and computational capacity becoming available, data-driven modelling of real-life systems is an increasingly popular approach both in the scientific community and industry. At the same time, there is a growing interest towards 'Digital Twins'; accurate, online and adaptable digital counterparts of physical structures which could be used e.g. as a design aid or to help with maintenance decisions at structures already in operation.

Universal differential equations (UDEs) [1] are a promising approach to include measurement data with machine-learnt structures inside differential equations alongside algebraic terms representing mechanistic models. By having a physics-based core, UDE models can incorporate the insight and expertise one has on the behaviour of the modelled structure. However, every physics-based model involves some degree of error compared to measurement data due to the dynamics neglected by the model. The purpose of using machine-learnable structures with the mechanistic model is to compensate the error between the observed and predicted behaviours resulting in not just a qualitatively but also quantitatively accurate model of the physical structure. While pure machine-learnt models could also be used for this task, the UDE model can be expected to require a smaller training dataset, more lightweight machine-learnt structures and, as a result, smaller computational effort as the physics-based part already stores information about the behaviour of the observed system.

Most of the studies on UDEs however focus on identifying a well-fitting model with a constant set of system parameters while it is often also interesting to investigate the system's response to varying parameters, e.g., to allow for parameter-uncertainty, or to incorporate the change of external conditions. Our study focuses on nonlinear dynamical systems and learning measured bifurcation diagrams using the UDE models leading to inherently varying-parameter problems.

Using the examples of aeroelastic flutter and a forced nonlinear oscillator [2] we assess the efficiency of the UDE modelling approach using neural networks [1] and Gaussian processes [3] as the machine-learnt part of the model. We demonstrate that the modelling approach has a great potential in delivering accurate models of nonlinear dynamical systems whereas we also report on the challenges encountered during the training procedure, such as overfitting and finding local minima of the objective function and discuss the potential ways of avoiding these issues.

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Pitch Bearing Parameter Estimation for Virtual Wind Turbine Testing Applications

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Key Words: *Virtual Testing, Parameter Estimation, Multibody Model, Kalman Filter*

Within the context of wind turbine component design, there is an interest to develop novel, advanced virtual test approaches using Digital Twins of both components and test bench setups. More specifically, virtual testing of novel pitch ball bearing designs is of interest, as these typically require large scale test setups.

In this work, the use of a Smart Virtual Sensing (SVS) Digital Twin [1] is proposed to estimate pitch ball bearing parameters, as well the overall system states and inputs. A multibody model of a pitch bearing test setup, including a parametrized analytical ball bearing model representing the pitch ball bearing, is combined with a Kalman Filter. A multibody formulation typically yields a set of Differential Algebraic Equations (DAEs) due to the presence of kinematic equality constraints. Recently, several approaches have been proposed in literature to combine these DAEs with a Kalman Filter ([1], [2] and references therein) for combined state and input estimation by relaxing the constraint definition leading to a set of non-linear Ordinary Differential Equations (ODEs). Rodriguez et al. [3] have recently presented an approach for multibody model parameter estimation. While these approaches cover equality constraints in different approximated ways, they do not in general consider inequality constraints. It is shown in this work that these approaches can lead to unstable behaviour of the Kalman Filter for bearing parameter estimation, as these parameters represent physical quantities, which in general have to be bounded (e.g. non-negative values) via inequality constraints. Without these constraints, the estimated parameter values can be out of bound and lead to unstable behaviour.

This work therefore further proposes an active set approach to enforce inequality constraints, stabilizing the Kalman Filter and allowing for robust bearing parameter estimation. The proposed approach is validated numerically and the necessity of including the inequality constraints to stabilize the Kalman Filter is highlighted.

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RL-ABC FOR MODEL SELECTION AND PARAMETER CALIBRATION APPLIED TO A NON-LINEAR EXPERIMENTAL TEST RIG THAT EMULATES A DYNAMICAL SYSTEM EVOLVING OVER TIME

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Key Words: nonlinear dynamics, parameter identification, model selection, reinforcement learning, ABC, decision under uncertainty

This paper proposes an extension of a recent developed methodology for model selection and parameter identification [1] which combines (i) reinforcement learning (RL) for model selection through a Thompson-like sampling with (ii) approximate Bayesian computation (ABC) for parameter identification and uncertainty quantification. Motivated by the digital twin framework where a system (physical twin) evolves over time, we consider three new features. (1) The worst model is not discarded because it might be useful in the future, as the system evolves. (2) The algorithm detects a change in the system by monitoring the models' acceptance; a significant drop in acceptance indicates a change. (3) If the system changes the algorithm is reset: new parameter ranges are computed and the Beta distribution of the Thompson sampling is restarted, as well as the rewards. Data are obtained from an experimental test rig which is a non-linear oscillator composed of a clamped beam with a tip mass, magnets and a coil. The amplitude of the dynamical system is obtained sweeping the amplitude of excitation; the control-based continuation strategy is used for this purpose [2]. The evolution of the system with time is emulated varying the distance between the tip mass and the coil. Three Duffing-like models are used: (a) cubic, (b) fifth-order and (c) seventh-order. Different cases are considered to test the new algorithm which seems promising for the analysed application and can be extended to others, for instance related to digital twin where a physical system is changing over time. The proposed RL-ABC strategy should be further tested in different systems to verify its extent.

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Robust State-Input Estimation for Differential Algebraic Equations and Application to Multibody Systems

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Key Words: *Kalman Filter, Multibody Model, State Estimation, Input Estimation, Digital Twin*

Digital Twins (DT) allow to accelerate the development of new products and enable new insights throughout the different product lifecycle stages. Smart virtual sensors based on DTs are capable of estimating quantities that cannot be easily measured, such as the full system states (and related quantities like strain and stress fields) and unknown inputs. Using a Kalman Filter approach [1], such a Digital Twin can be created by combining data coming from physical sensors with the asset's numerical model.

For complex mechanical systems composed of interconnected bodies and experiencing large motions and small deformations, a multibody formulation is commonly employed. The resulting equations of motion allow to efficiently express the kinematic constraints (i.e. connections) between the different components (i.e. bodies) using algebraic equations in combination with Lagrange multipliers. This yields a system of Differential Algebraic Equations (DAEs). Different approaches have been presented in literature to combine these DAEs (i.e. the multibody model) with a Kalman Filter ([2]-[4] and references therein). These approaches mainly differ in their handling of the algebraic constraint equations. They typically require using a specific multibody formulation and/or allow constraint violation (i.e. soft constraint enforcement). This tends to limit their use to either special cases or requires problem-specific tuning that can be detrimental for the application as a Digital Twin.

This work therefore presents a robust, general Kalman Filter-based state-input approach that allows to directly enforce the kinematic constraints exactly. More specifically, the estimated state is enforced to lie on the manifold described by the constraint equations and therefore meet the equality constraints exactly. This allows to generate a robust and smart virtual sensor using the Digital Twin of complex mechanical systems. The proposed methodology is numerically validated using closed and open kinematic chain multibody models.

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Stochastic Physics-based Model Updating for Fatigue Crack Detection in Riveted Lap Joints Using Lamb Waves

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Key Words: *Digital Twin, Lamb Wave Propagation, Fatigue Crack Estimation, Physics-based Model*

The mechanical joints (e.g., lap joint, weld, bolt, pin, etc.) are vulnerable to fatigue because of stress concentration and various internal flaws. Various digital twin strategies were used to support engineering decisions for system operation to prevent catastrophic system failure by fatigue damage in mechanical joints. The digital twin is a computational model that simulates the operating engineering system in the real world to support engineering decisions. The digital twin is a virtual model representing physical entities such as engineering products, components, and systems. The virtual model can be categorized into 1) data-driven, 2) physics-based, and 3) hybrid approach. The digital twin needs to be updated or analyzed using the observed response from the physical system to represent the current state/condition of the system. The PZT(lead zirconate titanate)-induced lamb wave is a suitable observed quantity for digital twin estimating crack detection in a mechanical joint. The PZT sensor is an active sensor in a fixed position, acquiring the repeatable signal without nonstationary noise. In a previous study, various data-driven approaches were proposed to estimate fatigue damage detection using PZT-induced lamb wave signal. He et al. (2013) proposed a data-driven approach to estimate crack length using Lamb waves in riveted lap joints based on the feature extraction and regression methods [1]. Pandey et al. (2022) proposed a deep-learning approach for damage detection using a 1-D convolutional neural network [2]. However, data-driven require many lamb wave signals measured in different crack lengths and geometry and suffer from low accuracy in noisy conditions. On the other hand, the physics-based approach is less dependent on data and is physically interpretable.

In this study, the stochastic physics-based model updating is proposed for fatigue crack estimation in riveted lap joints using lamb waves. The proposed approach is based on two techniques; (i) deterministic model calibration and (ii) stochastic model updating. In deterministic model calibration, physical properties of the medium, such as wave speed and decaying rate, are estimated using the observed signal. The k-Wave MATLAB Toolbox was utilized to simulate the lamb-wave propagation in the lap joint [3]. In stochastic model updating procedures, the possible crack growth path is sampled based on the probability of crack direction to consider uncertain crack propagation paths. The probability of the stochastic process is calibrated using Monter-Carlo simulation and the simplex method. The validity of the proposed method is demonstrated using an observed lamb wave in the fatigue test of the lap joint specimen. The results conclude that the proposed digital twin approach can accurately estimate fatigue crack growth state in lap joints.

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The Comparison of Sensor Optimisation Strategies for Structural Health Monitoring Using Machine Learning

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Key Words: Sensor Placement Optimisation, Supervised Learning, Unsupervised Learning, Time-series Data, Correlation Coefficient

Machine learning algorithms have been widely used to monitor the health of structures. The application of sensor placement optimisation (SPO) can be conducive to acquiring the most valuable data for constructing an effective damage identification model. There are two basic methods of machine learning, including supervised learning and unsupervised learning. The main difference between the two methods is whether to use labels of different structural health states. Therefore, different SPO approaches should be developed to improve the performance of structural health monitoring (SHM) systems based on these two machine learning methods.

In this paper, two SPO strategies with a linear correlation coefficient as the optimisation objective are proposed and compared using features extracted from time-series data. The critical difference between these two developed strategies is in whether the labels of different health states of a structure are involved in the optimisation process or not. A case study that uses the experimental data collected from tests on a glider wing demonstrates the characteristics of both strategies. The results show that the optimal sensor placement obtained by the first approach without considering the labels has better performance in detecting the occurrence of the damage on unexpected areas. However, if only the predictable damage cases of interest are focused on, the second optimisation approach that considers the state labels should be adopted.

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The Local/Global Coefficient of Friction of Elastic Contacting Bodies with Random Roughness

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Key Words: Isogeometric analysis, random roughness, coefficient of friction, frictional contact

In this paper, frictional contact problems of elastic bodies with random roughness are addressed using the Isogeometric analysis computational framework. To model the randomly rough surfaces, a new method is proposed consisting of a collocation-based Karhunen-Loeve random field modelling method and Non-uniform Rational B-spline (NURBS) interpolation method. The frictional contact problems are solved using a mortar-based contact algorithm. The local and global coefficients of friction (COF) are compared under the conditions of varying interfacial properties and external loads. The mean value and standard deviation of the global-to-local COF ratios of each scenario are obtained through Monte-Carlo simulations. Both quasi-static and dynamic contact problems are under investigation. It is found that the correlation length and Root Mean Square of the random contacting surfaces and the magnitude of the external loads impact significantly the development of global-to-local COF ratios with different rules.

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TRANSFER LEARNING TO LEVERAGE DIGITAL TWINS IN DRILL STRING DYNAMICS

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Key Words: digital twin, transfer learning, drill string torsional dynamics, localised friction, deviated wells

Digital twins seek to replicate a physical structure in a digital domain [1]. For a digital twin to have close correspondence to its physical twin, data are required. However, it is not always possible, or cost-effective, to collect a complete set of data for a structure in all configurations of interest. It is useful to repurpose data to help validate predictions for different configurations and scenarios. This is true in drill-string applications [2], where, for example, the length of the drill may be altered throughout operation. This paper demonstrates how transfer learning, in the form of three domain adaptation methods, — transfer component analysis (TCA) [3], maximum independence domain adaptation (MIDA) and geodesic flow kernel (GFK) — can be used to construct a digital twin for localising torsional friction in deviated wells under structural changes (e.g., when the drill column gets longer). The method uses a physics-based torsional model to train a machine learning classifier that can localise torsional friction for a given drill length, and diameter, where friction localisation labels are known (source). As the length or diameter of the drill are altered in the field, transfer learning is utilised to map the classifier from the labelled (source) scenario onto these unlabelled (target) scenarios. As a result, transfer learning improves the performance of the classifier when applied to the target data, and increases the domain of validity for the classifier. The performance of the classifier, and therefore its suitability to new drill configurations, is estimated by utilising two different distance metrics between the source and a proposed target dataset.

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A Parametric Reduced Order Model (pROM) for Structural Health Monitoring (SHM) relying on Ultrasonic Guided Waves

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Key Words: Parametric Reduced Order Model (pROM), Ultrasonic Guided Waves (UGW), Structural Health Monitoring (SHM), Damage Detection

Ultrasonic Guided Waves (UGW) bear an enormous potential for application within a Structural Health Monitoring (SHM) context. Advantages of UGW include their potential for detecting small defects, whilst propagating through long distances in thin structures, and the rather low cost of involved sending units (PZT-based). To unwrap the full potential of UGW, fusion of the measured data with models is required. Fused data and models allow for reaching higher levels of SHM – such as localisation or quantification of damage – following Rytter's specified hierarchy [1].

Due to their short period and wavelength, UGW require a fine discretization in time and space when one seeks to simulate the forward problem of wave propagation. This fine discretization leads to computationally expensive simulations. Since solving the inverse problem, which fuses UGW data with the models, necessitates repeated evaluations of the forward problem, the computational costs represent a major bottleneck towards effective use of UGW in SHM [2]. This work tackles this problem by introducing a parametric Reduced Order Model (pROM) for simulating UGW propagating in plates that contain flaws (e.g. cracks).

For efficient use, the pROM needs to be parameterized with respect to different defect configurations and properties, such as the location, shape or size of the defect. To train the pROM, enough information on the response of the system, depending on different parameter sets, is necessary. Due to the multiple parameters that can be involved, especially in the case of multiple flaws, and due to the large cost of the high–fidelity model, a sparse grid in the parameter space and additional knowledge on the systems behaviour needs to be used. To address this, we propose a pROM based on Gaussian Process Regression (GPR). The GPR enables to fit engineering knowledge through the definition of priors, while keeping the amount of high–fidelity training simulations low through active training. The developed framework is verified on simulated case studies.

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Damage detection in isotropic cracked rod via fusion of genetic algorithm with deep learning-based wave propagation simulators

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Key Words: Wave propagation, Damage detection, Structural health monitoring, Genetic algorithm, Inverse problem, Deep learning

Structural damage and deterioration of structures forms a primary engineering problem as such process can often cause catastrophic failures. The objective of structural health monitoring (SHM) is to identify anomalies or damages such as cracks, delaminations, etc. in structures. A number of SHM techniques exist for damage detection, such as vibration-based SHM, electromechanical impedance-based SHM, guided wave (GW)-based SHM, etc. The GW-based technique offers a number of advantages because of its high sensitivity to small defects and large area scanning. Damage detection is an inverse problem, in which the damage needs to be detected using the measured input and output signals. The conventional calculus-based search techniques use gradients, which can not handle problems having a finite number of discontinuities or functions with many local maxima or minima. But, genetic algorithms (GAs) can handle such problems without getting locked into a local optimum configuration. Damage detection in the form of an inverse problem can be performed using stochastic and evolutionary optimization methods, such as the GA, which is based on the principles of natural selection and genetic evolution.

In this research, elastic wave propagation emulated by a deep learning-based model is used as a tool for damage detection.The GA employs the deep learning-based simulator for multiple solutions of the forward problem. Our deep learning-based model is found to outperform traditional numerical solvers. Thus allowing low computational cost of damage detection, using GA as an optimization, with good accuracy.

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Full Waveform Inversion of Seismic Input Motions at a Domain Reduction Method Boundary in a PML-truncated domain

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Key Words: Inverse problems; seismic input inversion; non-convolutional second-order complex-frequency-shifted perfectly matched layers

A new inverse modeling is investigated for reconstructing seismic input motions propagating into a domain surrounded by a domain reduction method (DRM) boundary from limited seismic measurement data. The non-convolutional second-order complex-frequency-shifted perfectly matched layers (CFS-PML) is employed to truncate a two-dimensional semi-infinite domain of a plane-strain setting, and the DRM is utilized to model seismic input motions coming from the outside domain of the CFS-PML. A partial differential equation (PDE)-constrained optimization method aims at minimizing a misfit between measured motions at sensors on the surface induced by targeted incident waves (or equivalent effective forces on a DRM boundary) and their reconstructed counterparts induced by estimated effective forces.

The numerical results show that the targeted effective forces can be accurately reconstructed. It is observed that the wave responses in a structure and soils in the domain induced by the targeted effective forces are in excellent agreement with those by the reconstructed ones. Therefore, the presented method can help engineers to replay seismic responses of structures and soils from limited seismic measurement data and estimate the impact of earthquake waves on infrastructures.

Lamb wave-based damage identification in bounded structures through an inverse Bayesian process

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Abstract

Guided wave test is a promising technique for online monitoring in various industries such as aerospace and wind power. A Bayesian framework based on guided waves for damage identification of three-dimensional joints of arbitrary shape and finite size is presented here for the first time. The hybrid wave and finite element approach is adopted to obtain the scattering coefficients corresponding to different size defects, which can provide the results of different excitation types in a single operation. However, the physics-based Bayesian framework requires numerous calls to the physical model, which will drag the inversion framework into a time-consuming quagmire. In order to increase the efficiency of the proposed scheme, a Kriging surrogate model is used to generate a database containing measured scattering properties. Finally, a numerical model is used to validate the damage identification scheme.

Keywords: Guided waves, Bounded structures, Damage identification, Bayesian inference, Wave finite element, Surrogate model

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Simulation of wave propagation in remote bonded FBG sensors using the spectral element method

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Key Words: Wave propagation, spectral element method, optical fiber, FBG, non-matching mesh, remote bonding

Ultrasonic guided waves (GW) due to their ability to monitor large areas with few sensors, are commonly employed for structural health monitoring (SHM) in aerospace, civil, and mechanical industries. The FBG sensors in the edge filtering setup are re-emerging as a favored technique for GW sensing. The FBG sensors offer embeddability, ability to be multiplexed, small size, and immunity to electric and magentic fields and as such are seen as ideal sensors. To enhance the sensitivity of these sensors, these sensors are deployed in the so-called remote bonding configuration where the optical fiber is bonded to the structure while the FBG sensor is free. This configuration not only enhances the sensitivity but also opens up possibility of self-referencing.

In this setup the GW in the structure is coupled to the fiber and converted into fiber modes. These modes propagate along the fiber and then are sensed at the FBG. The conversion of the plate modes to fiber modes is a phenomenon which is still being studied. The effect of the adhesive layer and the material properties of the adhesive on the coupling are still not known. Furthermore the directional nature of this coupling and its marked difference from the directly bonded configuration needs to be studied in detail. For this detailed study a computationally efficient model which captures the physics of the coupling is necessary.

Hence, in this research we develop a numerical model based on the spectral element method for the modelling of the remote bonded configuration of the FBG. The model comprises four meters long optical fiber bonded to the centre of the plate by the adhesive layer and the piezoelectric disc (PZT) used for wave excitation. All components are modelled by 3D spectral elements, with second-order elements used for the fiber and adhesive layer. Parametric studies were performed for various thicknesses and the Young's modulus values of the adhesive layer, the FBG distance from the bonding fiber to the plate, PZT location and signal excitation frequency.

The model is validated with experimental results and shows that it indeed captures the physics of the coupling and is computationally more efficient than other methods using conventional finite element software.

Critical Velocity and Instability of Inertial Objects Moving Uniformly on Layered Track Models

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Key Words: *Moving Proximate Masses, Mass-Induced Frequency, Semianalytical Solution, Dynamic Interaction, Instability, Contour Integration*

In this contribution, a new form of semianalytical results related to inertial objects that are traversing homogeneous infinite structures, introduced in previous author's work [1], is used to analyze one-, two- and three-layer models of the railway track. The aim of these analyses is determination of the critical velocity of a moving force and of the onset of instability of moving masses or oscillators.

The new form of semianalytical results is related to infinite structures, but in addition to these derivations, equivalent finite models are presented and solved in order to provide easy validation of the results. For such structures, the eigenmode expansion method is used and therefore the natural frequencies and orthogonality conditions must be derived. Furthermore, due to the coupling of modal equations, a rearrangement of the terms involved is introduced to save computational time. All results, both from finite models and from infinite models, are presented as much as possible analytically using dimensionless parameters, and therefore can be used directly for several combinations of input data.

First of all, the possible range of dimensional parameters is identified. Within these ranges, there are significant differences between the models. While for the one- and two- layer models the critical velocities are well-defined and their number is 1 or 3 [1-3], respectively, in the three-layer model their number depends on parameter values and can be 1, 3 or 5. Regarding the onset of instability, there are also significant differences, not only between the models but also between the cases with one or more moving masses or oscillators. For one-layer model, which is in fact the model of an infinite beam on the classical Winkler-Pasternak foundation, instability of one moving mass has regular behavior and occurs always in the supercritical velocity range when damping is present and at the critical velocity in case of no damping. Two moving proximate masses already introduce severe alterations, because in damped case the dynamic interaction can shift the onset of instability deeply into the subcritical velocity range [2]. The other models introduce other irregularities, even for one moving mass [3]. This contribution will summarize all the differences and common features that exist between these models and within the full range of possible parameter combinations.

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15th World Congress on Computational Mechanics (WCCM-XV)
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A Generalized Beam Theory and its Applications in FGM Beam Structures

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Key Words: Generalized Beam Theory, Reference Beam Method, Stress Analysis, Functionally Graded Materials

Classical Beam Theories (CBT) are widely accepted as an efficient model to analyze mechanical properties of slender beam structures. They assume a rigid cross-section and neglect all stress components except axial normal and transverse shear stresses. However, the predictive quality of CBT deteriorates for stout beams and in a dynamic analysis, where in-plane distortions of the cross-section and the accompanied warping deformations become important. In such cases a Generalized Beam Theory (GBT) has to be used for realistic results. This talk discusses novel approaches in GBT [1, 2], where cross-sectional deformations are extracted from a modal analysis of a Reference Beam Problem (RBP). Each mode of the RBP is decomposed into a distortional and an accompanied warping field, and each individual part is then weighted axially within the member analysis by cubic shape functions. The resulting GBT formulation introduces three convergence related parameters, i.e., the number of elements discretizing the cross-section, the number of generalized beam elements and, crucially important, the number of introduced mode couples from the RBP. It is shown by example that the proposed model yields significantly better kinematical results compared to CBT, while the computational effort remains moderate. Additionally, detailed insight is given regarding the evaluation of three-dimensional stress distributions within the cross-section. It has to be noted that the proposed GBT formulation enables the introduction of inhomogeneous Functionally Graded Material (FGM) cross-sections by principle, and no further complexity is established regarding this modern branch of structural mechanics.

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A numerical analysis of magnetic heterogeneous microstructures based on micromagnetic finite element simulations

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Key Words: Micromagnetic Simulations, Finite Element Method, Microstructure

To cope with current issues such as the digitization, climate change and the turnaround in energy policy, new technological innovations will be indispensable. Here, particularly powerful and efficient magnets play a key role. A composition of magnetic grains and a decoupling non-ferromagnetic boundary layer can lead to an improvement in coercivity [1]. This shows the great potential of microstructure optimization. Here, numerical observations can provide support. Micromagnetic simulations are often combined with finite elements to determine the magnetization distribution on very fine scales. The latter are particularly suited for the precise geometrical approximation of very complex microstructures. The correct magnetic material behavior is captured by an enthalpy functional that contains contributions to the magnetostatic-, exchange-, anisotropy- and elastic energy. However, the evolution of the magnetization vectors is described by the Landau-Lifshitz-Gilbert equation. This equation requires the conservation of the magnetization vector length during the simulation. Since this is not fulfilled intrinsically, different methods of conserving the constraint have been developed, such as penalization strategies [2], exponential updates [3] or spherical coordinates [4]. In this contribution the results of finite element based micromagnetic simulations of heterogeneous microstructures are presented. Here, the focus lies especially on the analysis of their magnetic and mechanical material properties, the coupling between those fields and how they can be tuned by an optimal microstructure composition.

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Active Vibration Control of Aluminum Beam using Piezoelectric Actuator

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Key Words: *Piezoelectric Actuator, Beam Vibration, Active Control, PID Controller*

ABSTRACT

This paper deals with the active vibration control of the aluminum beam using a piezoelectric actuator. Cantilever beam was excited by one thin piezoelectric film placed near the fix support. [1] The second piezoactuator was placed near the first one and used for active vibration suppresion. The oscillation of the beam's free end was measured using a laser position sensor.

The beam's eigenfrequencies and damping ratios for the first and second bending vibration modes were determined using FEM and verified experimentally. These results were used to design simulation model of the control system with PID Controller.

The excitation actuator was driven by signal generator to produce forced vibration of the system. The control actuator was driven by DAQ device and controlled using LabVIEW software. The excitation and control actuators were powered by high-performance power supplies and linear amplifier modules.

The operation of the designed control system for damping free as well as forced vibration of the cantilever beam is finally evaluated.

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Analysis and Testing of Modular Functionally Graded Soft Metamaterial

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Key Words: *Soft Materials, Wang Tiles, Metamaterials, Testing, 3D printing, Open Hardware*

Soft materials and metamaterials explicitly are going to be a key paradigm for industrial applications, as e.g. soft robotics, medicine and/or collaborative technologies, of the 21st century. In this contribution, we discuss the use of the Wang tiling based modular concept in the design, manufacturing, and self-assembly of a soft graded metamaterial for soft-robotic scissors-like gripper, and its testing by means of in-house small scale portable testing frame.

The talk splits into two parts. The first part addresses the tiling concept in its most straightforward installment, the design a soft porous metamaterial with a non-periodic structure and its manufacturing. Here, the emphasis is put on the inherent modularity of the concept and a potential for scalable robot-assisted sample production.

The second part aims at an Open Hardware based high precision mechanical testing frame for experimentation on small-to-medium size soft material samples under the loads up to 50N supported by the contact-less DIC measurement system. The frame has been specifically tailored for testing soft (meta)materials as that discussed in the previous part, namely in horizontal setup to exclude the gravitational forces acting on two-dimensional experimental specimens and causing unwanted out of plane buckling. Despite its primary purpose, it has finally developed into a powerful self-sustained experimentation system that may be used in several ways in different engineering disciplines in both vertical and horizontal setup.

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Analysis of Actuator Structure Using New Electro-Thermo-Mechanical Finite Element Derived for Functionally Graded Materials

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Key Words: *New Finite Element, Functionally Graded Materials, Multiphysical Analysis, Actuator*

Functionally Graded Materials (FGMs) are new types of material where their properties vary spatially according to chosen function to reach such features that are unable to provide using standard materials or composites. Hence, a structure made of FGM can dispose for example with excellent thermal conductivity at one component part together with thermal insulating properties at another component part.
Proposed paper deals with electro-thermo-mechanical analysis of chosen actuator structure made od FGM using new finite element derived specially for this purpose. Rectangular cross-section of individual beams that form the von Mises structure with variation of material properties in longitudinal and lateral direction will be considered. Actuator action, electric voltage and temperature peak and also mechanical stress of the structure will be evaluated. Results from the analysis calculated using our new FGM beam finite elements will be compared to results from conventional FEM analysis where standard finite elements will be used.

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Beam Finite Element with Piezoelectric Layers – Modeling and Control

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Key Words: Finite Element Method, Piezoelectric Analysis, State-Space Model, LQR Control, MOR

Smart materials are a very important building blocks in mechatronic applications [1]. These materials include shape memory materials, magnetorheological, functionally graded, piezoelectric, and other types of modern materials [2] . Their main feature is their possibility to extend the functional usage of a given system, to modify the dynamic behaviour of a given system or to allow a return to the original state of the system under certain conditions.

The paper deals with the development of the finite element method (FEM) model of piezoelectric beam elements, where the piezoelectric layers are located on the outer surfaces of the beam core, which is made of functionally graded material. The created FEM model of piezoelectric beam structure is reduced using the modal truncation method, which is one of model order reduction (MOR) method. The results obtain from reduced state-space model are compared with results obtain from finite element model. MOR state-space model is also used in the design of the linear quadratic regulator (LQR). Created reduced state-space model with feedback with the LQR controller is analysed and compared with the results from FEM model.

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Warping Torsion of FGM Beams with Open Cross-section and Spatially Varying Material Properties

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Key Words: *Warping Torsion, FGM Beams, Spatially Varying Material Properties*

In this contribution, which is an extension of author's research [1, 2], the influence of the in three directions varying material properties on non-uniform torsion of Functionally Graded Material (FGM) thin-walled beams with open cross-section is originally investigated. The effect of warping and secondary deformations due to the angle of twist is considered. The warping part of the first derivative of the twist angle caused by the bimoment is taken into account as an additional degree of freedom at the beam's finite element nodes. The Reference Beam Method (RBM) [2] is applied for homogenization of the spatially varying material properties in the real beam towards effective longitudinally varying stiffness quantities. The focus of the numerical investigation, with consideration of the warping and Deformation Effect due to the Secondary Torsional Moment (STMDE), lies on elastostatic torsional analyses of straight FGM cantilever beams with open I-profile cross-sections. The influence of the variation of the material properties with respect to three directions on the angle of twist, the bimoment normal and the torsional shear stresses, respectively, is investigated. The obtained results for primary and secondary variables are compared with the ones calculated using very fine meshes of standard solid finite elements. A large influence of the variability of material properties on the deformation as well as on the stress state of the beam with I-cross-section, calculated by the author´s FGM WT beam finite element has been found. The entire real beam with spatially varying material properties is modelled by only one FGM WT beam finite element, thus the proposed algorithm causes only very litle computational effort.

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Code-Oriented Floor Acceleration Response Spectra of RC Framed Buildings Accounting for Nonlinear Response of Masonry Infills

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Key Words: *Floor Acceleration Response Spectra, RC Framed Buildings, Masonry Infills, In-Plane and Out-Of-Plane Response, Nonlinear Seismic Analysis.*

Damage surveys that followed the occurrence of strong earthquakes have shown that code provisions may result in wrong estimation of the safety of masonry infills (MIs), which is generally carried out through simplified methods. The types of damage observed for MIs are usually a combination of, or an interaction between, in-plane (IP) and out-of-plane (OOP) mechanisms. The IP drift ratio is generally reduced at the upper storeys of buildings, where the OOP drift ratio increases due to an increase of seismic acceleration. Significant OOP damage may also take place at the lower storeys where the highest values of IP drift ratio are attained. The present work is aimed at identifying the effects of the IP and OOP nonlinear modelling of MIs and their mutual interaction on floor acceleration response spectra. To this end, a spatial one-bay multi-storey shear-type model is considered as equivalent to infilled RC framed buildings, having MIs made with two 12 cm leaves of clay hollow bricks. Additional variability of the following design parameters is considered: number of storeys (three, five and seven); behaviour factor (low, 1.5, medium, 3, and high, 4.5); OOP strength of MIs, with lower and upper bound values corresponding to one- and two-way arching mechanisms, respectively. A recently proposed computer code including a five-element macro-model [1], comprising four diagonal OOP beams and one (horizontal) central IP truss for nonlinear modelling of MIs, is considered for the numerical investigation. The proposed algorithm modifies stiffness and strength values of MIs in the OOP direction on the basis of simultaneous or prior IP damage and vice versa. Moreover, a lumped plasticity model describes the inelastic behaviour of RC frame members. Biaxial spectrum-compatible accelerograms are considered at life-safety limit state provided by the Italian seismic code. A simplified code-oriented formulation for the assessment of floor response spectra of infilled RC framed structures is proposed. Nonstructural maximum acceleration is firstly evaluated by means of vertical and nonstructural amplification factors. Continuous wavelet transforms are used to calibrate parameters that define the resonance region width, accounting for moving resonance due to nonlinearity and higher modes effects. Parabolic and Gaussian curves are considered in order to reproduce pre- and post-resonance regions, respectively. Finally, code-oriented proposal is compared to exact floor spectra of MIs evaluated in the common range of OOP vibration periods (i.e. 0-0.3s).

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Mitigation of Seismic Pounding between Adjacent Buildings by means of Isolation and Supplemental Dissipation at the Base

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Key Words: *Seismic Pounding, In-Plan Irregular Structures, Near-Fault Site, Single and Double Concave Surface Sliders, Viscous Dampers.*

Double concave surface slider (DCSS) is considered as an effective solution for base-isolation of existing structures located in a near-fault site, because of its capacity to notably increase horizontal displacements that can be accommodated in comparison to a single concave surface slider (SCSS) of identical in-plan dimensions. However, unexpected torsional pounding of in-plan irregular adjacent structures may be induced by variability of frictional force and lateral stiffness of both SCSS and DCSS, depending on the axial load and friction coefficient changes during an earthquake [1]. Effectiveness of supplemental viscous damping at the base is studied in this work with the aim to analyse its effectiveness for limiting base displacement, so avoiding too large seismic gap requirement. To this end, structural pounding between fixed-base and base-isolated L-shaped buildings, placed adjacent to form T- and C-shaped plans, is analysed. A simulated design of the original reinforced concrete (RC) fixed-base framed structure is preliminarily carried out in accordance to a former Italian code, for a medium-risk seismic zone and a typical subsoil class. Then, seismic retrofitting with SCSSs is carried out, in order to attain performance levels imposed by the current Italian code in a high-risk seismic zone and for moderately-soft subsoil, while DCSSs have radius of curvature equal to half the SCSSs and the same friction coefficient. Different in-plan distributions of linear fluid viscous dampers (FVDs) are examined, following damping distribution inversely proportional to the distance between the stiffness centre of the base-isolation system and the plane frame where each FVD is placed. Moreover, the equivalent viscous damping ratio of the supplemental FVDs is taken in the range 10%-20%. Nonlinear modelling of SCSSs and DCSSs considers variable axial load combined with friction coefficient at breakaway and stick-slip and as function of the sliding velocity, axial pressure and rising temperature at the sliding interface. Attention is focused on the pulse-type nature of near-fault earthquakes generally observed in the velocity time-histories but largely overlooked in the acceleration ones. Automated classification algorithms using wavelet analysis are adopted to compile three datasets of seismic input rotated in the range 0°-360°, with a constant step of 15°. Distinction is made between no-pulse and velocity-pulse, the latter further categorized into non-acceleration and acceleration-pulses. Combination of DCSSs and FVDs results the most suitable trade-off between mitigation of maximum response of the isolation system and seismic pounding between adjacent fixed-base and base-isolated structures.

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Using transit finite element method to evaluate the Structure-borne noise levels of metro system bridges

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Key Words: *Structure-borne noise, Metro, Vibration, Finite element method*

Taipei is home to a 146-km-long metro system that handled a record number of 1.9 million passengers in a single day in 2020. At present, approximately 56% of the Taipei metro network is composed of bridge structures, and in the following decade, bridge structures are expected to double in length within the Taipei metropolitan area. However, the problems caused by noise and vibration pollution are also on the rise as the Taipei metro expands further using viaducts

The structure-borne noise problem is a coupled problem that involves both noise and vibration. Most metro-related noise studies have focused on high-frequency and low-frequency noise, and structure-borne radiation noise has rarely been studied. For this reason, this study discusses the relationship between the local vibration of bridges and the structure-borne noise. Then, a transit finite element method (FEM) is applied to model the train–track–bridge dynamic interaction problem and evaluate structural vibration.

Three of the most common types of bridges, i.e., double-box pre-stressed concrete (PC) girder, double-box steel girder, and double-U-shaped PC girder are investigated in this study via in situ measurement and 3D transit finite-element analysis. The effects of plate thickness, trackpad stiffness, train speed, and track irregularity on bridge plate vibration are considered in this study. Finally, the proportional evaluation method is proposed and a structure-borne noise influence index is used to determine efficient methods to reduce structure-borne noise.

The conclusions show during the bridge design stage, the best combination of thickness and rail stiffness can be chosen to reduce the local vibration. Each bridge type can modify the rail stiffness to reduce the structure-borne noise index. In the operation stage, the methods of reducing the structure-borne noise would be to change the train speed and grind the rail to make the rail running surface smoother. In the viewpoint of reducing structure-borne noise, the PC box girder is the most commonly recommended bridge type for use in urban areas, and it generates the lowest vibration levels among the three types for each parameter combination.

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An efficient data-driven model reduction approach for multiscale homogenization of a microstructure with hysteretic mechanical behavior

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Key Words: *Microstructure, Data-driven approach, Artificial Intelligence, Surrogate model*

Composites have become the most promising materials of this century applied in a variety of engineering fields including aerospace, automobile, and marine by their merits of high strength, and lightweights. In addition, most composites have heterogeneous characteristics, consisting of two or more different phases such as matrix and inclusions, at the microscale. Therefore, computational homogenization method has been a favourable approach to describe an effective continuum model for heterogeneous composites at the microscopic level. Also, it can be extended for a multilevel finite element method known as the FE^2 method. However, heterogeneous composites with hysteretic nonlinear behavior causes significant computational cost and inevitable many-query simulation due to the complex deformation mechanisms while connecting different scales. From this point of view, the reduced-order model can be an appropriate approach to overcome those significant drawback related to the computational inefficiency [1]. In this study, we propose a surrogate model that can efficiently predict the global and local nonlinear behavior of microstructure by applying a deep learning-based data-driven model reduction method. Herein, variational autoencoder (VAE) can be applied for a model order reduction method based on a deep neural network [2]. It is utilized to handle the quantities of interest on the RVE of microstructure. Moreover, we employed a gated recurrent unit (GRU) to describe the hysteretic relationship between stress and strain [3].

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An efficient DNN-based Data-Driven Modeling algorithm for the Real-Time Flexible Multibody dynamics

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Key Words: Flexible multibody dynamics, Deep neural networks, Stochastic graident descent, Error correction, Real-time simulation

Predicting system responses in real-time have been required in various industries. A deep neural network (DNN) based data-driven modeling have shown the possibility without compromise accuracy for the highly nonlinear systems. In the rigid multibody systems, without solving the equations of motion of the systems, well-trained DNN model can predict the responses in real-time with high accuracy [1].
In this study, we introduce a data-driven metamodeling technique to deal with the multibody systems with flexible bodies. To handle the huge data which are come from the degrees of freedom of the flexible bodies, an efficient two-step training algorithm has been presented [2]. In the first step of the algorithm, a stochastic gradient descent (SGD) step, several coarse data sets are constructed by selecting randomly from the full data. The initialized DNN model is trained sequentially and iteratively with the coarse data sets. When improvement of the model accuracy from the iterative training is not sufficient, it moves on to the error correction step. In the EC step, a DNN model that predicting the error of the DNN model obtained in the final step of the SGD step is trained. The final predictions are calculated as the sum of the prediction of the SGD model and the error predicted by the EC model.
Through the proposed algorithm, it is possible to train a DNN model that uses only a part of the full data to increase the training efficiency and predicts accuracy similar to the trained model using the full data. The performances of the proposed algorithm have been verified using some numerical examples. It is confirmed that the DNN model can obtain the desired responses in real-time.

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Deep learning-based Approach for prediction of Airfoil Aerodynamic Performance in Low Reynolds number

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Key Words: *Convolutional Neural Network, Airfoil, Aerodynamic characteristics, Autoencoder, Proper Orthogonal Decomposition, Signed Distance Function,*

Interest of aerial vehicles such as a small Unmanned Aerial Vehicle(UAV) and Micro Aerial Vehicle(MAV) has risen during the last few decades. Many of these aircrafts use a fixed wing or rotor blade and operate at low Reynolds number regime. For example, *Re* is commonly less than 2×10^5 or 1.5×10^4 for MAVs or Nano Aerial Vehicles(NAVs), respectively. Moreover it can be even lower for insect flight [1]. For the design of the wings or blades of these biomimetic aerial vehicle or a drone for atomospheric planet exploration, the unsteady blade element momentum theory can be employed. Herein, aerodynamic performance of an airfoil at low Reynolds number should be considered [2]. In general, evaluation of aerodynamic performance of airfoil can be performed by mean of Computational Fluid Dynamics(CFD). Recently, studies applying machine learning to reduce the computational cost and time of CFD are being conducted [3]. In this study, a framework based on deep learning technique is proposed, which can predict the aerodynamic performance of airfoil at low Reynolds number regime. The input of the network is the airfoil data represented through Signed distance function(SDF), and the output is the pressure field of airfoil. To improve an efficiency of the proposed framework, three model-order reduction methods, i.e. proper orthogonal decomposition(POD), autoencoder (AE), and variational autoencoder (VAE), are considered to describe the pressure field of the airfoil.

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Exact Model Reduction of Nonlinear Finite Element Models via Spectral Submanifolds

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Key Words: Model order reduction, Invariant Manifolds, Nonlinear Finite Elements, Normal Forms, Nonintrusive methods, Direct methods, Forced Response Curves, Backbone Curves, Isolas

Finite element models of realistic nonlinear structures are characterized by very high dimensionality that renders simulations of the full system infeasible. Mechanical structures are usually characterized by light damping which results in exceedingly long integration times before a steady state is reached. Despite the broad availability of dedicated software packages, the computation and continuation of the steady-state in response to periodic forcing remains a serious computational challenge for full-scale nonlinear finite element models.

The recent theory of Spectral Submanifolds [1] has laid the foundation for a rigorous model reduction of such nonlinear systems, leading to reliable steady-state response predictions within feasible computation times. Further developments [2] have enabled the computation of SSMs and their reduced dynamics by solving the associated invariance equations directly in physical coordinates using only the eigenvectors associated with the master modal subspace. The software implementation of the method has been available in an open-source package, SSMTool [3], making direct SSM computations scalable to realistic, nonlinear finite-element models.

In this talk, we demonstrate recent advances towards the computation of SSMs that enable the treatment of realistic finite-element models using direct as well as non-intrusive/data-driven methods.

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Further Evaluation on the Projection-based Model-order Reduction Considering the Nonlinear Properties

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Key Words: *Projection-based model-order reduction (PMOR), Proper orthogonal decomposition (POD), Hyper-reduction, Defect-parametric reduced-order model (Dp-ROM)*

For the mechanical and aerospace hardware, e.g., turbine blade, aircraft wing, large-size dynamic simulation which uses huge computational resource and iterative computation will usually be required for their fluid-structure interaction (FSI) and design optimization while considering their nonlinear properties.
In this paper, projection-based model order reduction (PMOR) technique will be suggested and applied to reduce the relevant computational expense.
PMOR is one of the traditionally intrusive approaches to construct a reduced-order representation by directly projecting the full-order representation onto a lower-dimensional subspace or reduced-order basis. The proper orthogonal decomposition (POD) [1] is a representative data-driven method, and it has been a widely used technique under the idea of PMOR. However, its recursive projection process for a nonlinear simulation may incur a significant computational expense. To compensate such computational inefficiency, the POD-based reduced order model (ROM) will be suggested and combined with the hyper-reduction technique [2]. The present hyper reduction includes the discrete empirical interpolation method, Gauss-Newton with approximated tensor, and energy-conserving sampling/weighting. It will allow reconstruction of the nonlinear terms in the reduced dimension, by using smaller number of the sampling points. Furthermore, a defect-parametric reduced-order model (Dp-ROM) [3] based on the modal method [4] will be applied to efficiently address the parametrized shape defects.
The aim of this paper will be to develop various projection-based ROMs and systematically evaluate the resulting ones regarding the prediction capability for the nonlinear formulations accurately and fast. To achieve such goal, numerical examination will be conducted regarding the time-transient analysis for an aircraft propeller and wing which possesses geometrically nonlinear characteristics.

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Improved Parametric Model Order Reduction for Fluid-structure Interaction

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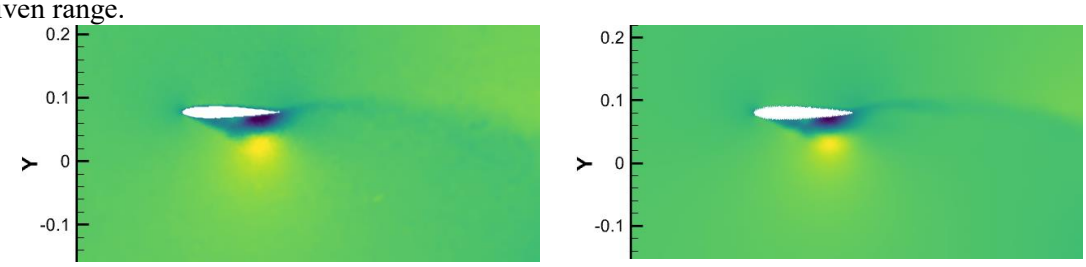
Key Words: *Machine Learning, Convolutional Autoencoder (CAE), Variational Autoencoder (VAE), Fluid-structure Interaction (FSI), Model Order Reduction (MOR)*

In this abstract, an improved machine learning-based model order reduction scheme is presented for the parametric estimation regarding the fluid-structure interaction (FSI) problem. The current scheme consists of the following two stages: spatial and temporal reduction on the computational fluid dynamics (CFD) flow field. The first stage is done by the convolutional autoencoder (CAE) which significantly reduces the number of DOF for the flow-field. The second stage is by the variational autoencoder (VAE) which reduces the number of DOF's in the temporal space.

The current scheme is then applied for a simple FSI situation on a two-dimensional NACA 0012 airfoil. The airfoil of a chord length of 0.156m is subjected to a uniform flow in a standard atmosphere at the incoming flow speed of 1m/s. The airfoil is also subjected to the prescribed plunging motion with the plunging frequency of 10rad/s where the plunging amplitude varies between 0.05 and 0.14m in 10 increments [1]. The full-order model (FOM) snapshots are obtained by Navier-Stokes CFD analysis, OpenFOAM v1912.

From the snapshots, the latent codes for the first stage are constructed for each parameter and time step by using CAE. The latent codes for the first stage contain the temporal and parametric information in a reduced form (spaital information reduced into several codes) and are provided to the second stage. VAE then will reduce the first latent codes and temporal information into the second stage latent codes which will contain only the parametric information. Afterwards, the second latent codes will be interpolated and fed back to the decoders of VAE and CAE in order, while constructing the interpolated flow field.

As a result, the interpolated flow field for the plunging airfoil of 0.095m will be constructed. The average flow field velocity discrepancy is found to be as small as 0.23%, as shown in Fig. 1. For the present approach, the offline stage requires 75.6 hours for ten FOM constructions by using CFD. The training for CAE and VAE requires 29 hours. The online stage, composed of executing the interpolated latent code through the decoders requires smaller than 0.2 hours. The current scheme will become more efficient when more than four interpolated flow fields are to be required for the given range.



(a) Interpolated flow field (b) Full order model

Fig. 1. Original and interpolated flow field using the current method

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Model Order Reduction of Coupled Problems in Structures

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Key Words: *Model order reduction, Coupled field problems, Modal vectors, Krylov subspace*

The finite element discretization of coupled partial differential equations leads to complex and very large-scale discretized equations [1]. The time dependent analysis of these large-scale coupled discretized equation is computationally challenging. Generally, the projection-based model order reduction methods are used to get computationally efficient solutions of large-scale dynamical systems. In this work we use a method based on sequential projection which was proposed by Kim et al. [2] for the model order reduction of strongly coupled problems. Thermomechanical coupled systems are considered for the study. First the modified mode superposition method based on modal vectors is used to obtain the reduced order models of thermomechanical systems. In the next part, projection matrix obtained from Krylov subspace technique is used for model order reduction of the thermomechanical coupled systems. The numerical accuracy and computational efficiency of the model order reduction methods is studied for different thermomechanical systems.

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Prediction and Validation of the Dynamic Characteristics of 3D Rotor Blades using Convolutional Neural Networks with Image Composition

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Key Words: *Prop-blade, Natural frequency, Fan-plot, Convolutional neural networks*

In this work, a convolution neural network (CNN) was employed to construct a surrogate model to represent the dynamic characteristics of prop-blades, such as fan-plots in terms of natural frequencies, according to the rotational speed of the rotor. A set of key images of the cross-sections of a rotor blade whose outer mold layer (OML) was determined by aerodynamics designers. The cross-sections images were illustrated with individual color pixels according to the spar, skin, and OML, which also expresses the structure of the cross-sections of the blade. After converting color pixels into grayscale images, as input data of the CNN model, 1000 image sets consisting of 10 cross-sections of the rotor blades were adopted. As output data, 1000 fan-plots were prepared. During the training, 93% of the data set was used for the training, and prediction of the fan-plot of the blades was conducted with 7% of the data set. Twenty CNN models were created to find the model with the best performance. To demonstrate the performance of the proposed CNN model, we predicted the dynamics characteristics in terms of the fan-plots on various test data sets. The prediction accuracy was verified in terms of the loss functions and the error of the natural frequencies. The prediction results were in excellent agreement with the test data sets, and the fan-plots were quickly predicted for other rotor blade cross-section images. This confirmed that the proposed CNN model is simple and powerful and can efficiently clarify the relationship between the rotor blade cross-section images and fan-plots of rotor blades.

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Study on Damage Detection Technique based on eXplainable Artificial Intelligence and Validation via DIC Experiment

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Key Words: *Damage Detection, eXplainable Artificial Intelligence, Class Activation Map, DIC*

When damage occurs to structures, such as the wing of aircraft and blades of rotorcraft, it is generally initiated in local and spread to the entire structure. To prevent the destruction of the entire structure due to the damage occurring in a local area, it is important to detect and act on damage at an early stage through real-time monitoring of the entire structure [1]. Techniques for detecting structural damage include modal based detection techniques and strain-based detection techniques. However, these techniques can change the dynamic characteristics of a structure by attaching a sensor to the structure and it may require large amount of sensor to increase detecting resolution. To compensate for those shortcomings, research on displacement/strain measurement using a non-contact method, Digital Image Correlation (DIC) [2], has been conducted. DIC is a technique to measure the deformation and displacement of a structure using images before and after the deformation of the structure. In addition, it is relatively straightforward to achieve the real-time monitoring of the structures by using the DIC equipment. In this paper, a method for monitoring the presence or absence of damage and the location of damaged area is developed by using the Class Activation Map (CAM) network, a kind of explainable artificial intelligence technology. To generate training data, the finite element method is used to obtain displacement/strain of a target structure. The developed CAM network can classify the presence or absence of damage by considering the strain fields. Moreover, the relevant result of the CAM network is the CAM image which indicates a damage location of the structure. Finally, the present CAM network for damage detection will be validated by considering the DIC experimental data of tensile specimens.

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A new crash absorbing origami structure RTO and comparison of RTO with origami structures with 4 folding lines at intersection

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Key Words: *RESERVED SPIRAL ORIGAMI STRUCTURE, REVERSED TORSION ORIGAMI STRUCTURE, PARTIAL-HEATING TORSION MOLDING METHOD,HALF CUT SEMI ORIGAMI STRUCTURE , LIQUID PRESS FORMING METHOD, POLYGONAL CROSS SECTION SEMI ORIGAMI STRUCTURE*

In the crash collision, the vehicle energy absorbers play an important role in the energy absorbed performance. Current vehicle energy absorbers have two defects during collision, such as only 70 % collapsed in its length and too high initial peak load. It is because present energy absorbed column is the most primitive from the point of Origami structure. We developed the column so called Reversed Spiral Origami Structure; RSO which solves these 2 defects[1]. However, for RSO, the manufacturing cost of hydroforming[2] in the existing technology is too expensive to be applied in real vehicle structure. To address the problems, we have developed a new forming method called "Partial-heating torsion forming method". And we have developed RTO (Reversed Torsion Origami Structure) by this new forming method at a very low cost[3]. We show this RTO also solves the two defects of the present vehicle absorbers by not only simulation but also experiments. This structure is possible to replace conventional energy absorbers and it is expected to be widely used such as not only in automobile structures but also in building ones. By the way, there are 3 types of crash energy absorbing origani structures such as RSO & RTO which have 6 folding lines at each intersection , bellows hold which has 4 folding lines at each intersection and semi origami structures such as , Also it is discussed advantages and disadvantages of these three types of origami structures.

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Development of New sound insulation simulation technology using Finite element method and its application to Origami core

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Key Words: *Origami Forming, Incident Wave, Reflective Wave, Optimization*

We have developed a new truss core panel by origami forming to get the higher aspect ratio than that by multi-stage press forming. Our object is to apply the new origami truss core to the train floor. Whether or not this goal can be achieved depends on whether this new origami truss core with a high aspect ratio has excellent sound insulation characteristics especially in low frequency range. Therefore, to estimate accurately the relation between the aspect ratio and the sound insulation performance, we try to develop an effective simulation technology with finite element method (FEM). So far, sound insulation simulations using FEM did not match with theory of the mass law [1]. However, this can be achieved by setting the end of the transmitted side to be a nonreflective boundary for a panel that is supposed to be stiff enough [2].

In this paper, to generalize this method, it is determined theoretically that the sound pressures from the FEM can be separated accurately into the sound pressures of the forward and backward waves from Helmholtz's equation. In addition, the validity of the proposed method is confirmed by evaluating the effect of attaching a sound absorbing material to the plate. Furthermore, application of the proposed method to a flat plate with one core and an examination of whether a high aspect ratio is advantageous for sound insulation are also presented.

In addition, with this method, it is confirmed that the shape to optimize the sound insulation performance under certain conditions canbe calculated because the knowledge that the sound insulation performance in the low frequency range improves in the flat plate with a high aspect ratio vertical core was obtained. As a result, it is expected to improve the sound insulation performance of low frequencies that cannot be compensated with sound absorbing materials.

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Origami metamaterial reconstructing any structure including non-convex curved surface in a row

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Key Words: *Origami Forming, Incident Wave, Reflective Wave,Optimization*

Nojima and Saito introduced the term “kirigami honeycomb” in [1] where they use the cross section of the 3D shape to describe the panel and include cuts in the pattern to obtain its 3D structure. Neville et al [2] have studied the mechanical properties of “kirigami-honeycomb” panels to test its feasibility of using shape memory polymers (SMPs) to actuate the folds in open Kirigami-honeycombs. Recently, Caslish and Gershenfeld [3] designed a continuous folding machine to construct the Kirigami patterns obtained by the previous method [1]. However, above approaches [2, 3] also use two curves in the cross section of the shape that limits the representation of shapes with more complex geometries.

In our proposal, the design method is generalized for more complex shapes based on 3 fundamental contributions: 1) the need to represent the shape by 2 curves in the cross section to represent any 3D shape is eliminated, 2) the ”honeycomb cores” are embedded in the 3D shape by means of boolean operations on the 3D shape and 3) an optimal method of assigning folding lines, cutting and gluing areas was developed for the manufacturing of the panel.

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Origami to Decode Folding Strategies in Nature

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Biomimetics, is in essence learning from and mimicking, emulating the strategies, formations, systems, structures and etc. found in native biological systems. Among several strategies in nature, folding which can be observed in biotic and abiotic part have been studied extensively. Folding is not “an adaptation but merely a physical consequence that just emerged at a point in evolution”(Hunter 2015)

Folding is determined by force and material as shown by Kresling (2012), Miura (1997), Yoshimura (1951 changing the structural memory of material by exceeding the yield point. Paper for example, is an excellent medium to understand folding where a crease is a plastic deformation of the sheet, where it has passed the yield point, “effectively re- setting the elastic memory of the paper to a non-zero angle” (Demaine et al., 2009). Understanding the “fold memory of materials/matters” result in many new models in several disciplines like biology, robotics, space structures and many novel solutions in use of shape memory alloys and today in developing 4-D printing for which shape shifting is achieved not only by the material but also by the form.

Architecture like many other fields deeply involves in biomimetic research to find novel solutions in the design problems. Responsiveness which is a broad term employed to explain force-artefact interactions under external forces or internal forces related uses folding as a strategy to optimize the performance through kinetic systems. In this paper, how origami and biomimetics are employed in developing novel solutions in architecture is to be discussed. First recent advances in biomimetics and origami used in architecture is to be scrutinized, then examples developed within this framework through the projects in METU are to be explained showing how thick folding and 4-D printing is used not only as form finding of kinetic surfaces, but also solving mechanisms either for modular or tessellated structures as well as new potentials to develop recursive kinetic formworks.

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"Proposition of a new "Energy density topology optimization method for eigen frequencies" and its application to origami safe carrier box

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Key Words: *Space Filling, Control of Plural Eigenfrequencies, INDEX OF GENERALIZED EIGENFREQUENCY*

No solution has been obtained for situations where fruits and vegetables such as strawberries, cells, blood, etc. are damaged or die during transportation. It is presumed that the biggest factor in these situations is that there is a perishable and mortal vibration band. For example, the frequency band that most affects ride comfort of train and car passengers is said to be 4 to 10 Hz. Therefore if there are eigen frequencies of vibration system consisting of seats, floors, and occupants, it is designed to move out of band with resonant frequencies. In this study, we will examine the basic issues for the challenge of moving the resonance frequencies to solve the above-mentioned problems of damage and death of fruits and vegetables and cells. The birth of topology optimization analysis technology was expected because generally speaking, significant movement is difficult to move of resonance frequency with dimensional optimization but realization of topology optimization was not easy. Since the topology optimization was finally developed using the homogenization method in 1988[1], so much research of topology optimization has been done.

Tenek and Hagiwara compared for static problems between using each element thickness as design variables and homogenization and showed that there was no big difference[2]. Now the former is called the density method and the density method is now more commonly used than the one using homogenization. Now since reference [1], the second author Hagiwara also published some papers concerned with topology optimization. Judging based on these experiences, the conventional topology optimization methods cannot be easily applied to the problem of lowering some resonance frequencies and raising some resonance frequencies.

Although this idea can be said in common both for static stiffness problem and for dynamic vibration problem. Therefore, we propose here a new method named "Energy Density Topology Optimization Method" which has been discovered by returning to the origin of vibration where eigen frequency is determined by equivalent stiffness and equivalent mass. And also shown is the origami safe carrier box by this new method.

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Numerical Modelling of Influence of Interface Properties on the Performance of Interpenetrated Composites

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Key Words: *Metal-ceramic Interpenetrating Phase Composites, Impact Loading, Peridynamics, Finite Element Method, Atomistic Simulations*

Multiphase Ceramic Composites (CCs) are used in several modern industries like aerospace, automotive, nuclear power, or defense. They are used in the situation of expected extreme loads like variable loads or impacts.

The interpenetrating composites (IPCs) is a class of composites that are defined by the technological process. The IPCs consist of a crushable skeleton and a metallic phase introduced into the skeleton under pressure. The resulting material combines the features of the skeleton and the filling metal.

Earlier analyses of the composite systems showed the significance of the interface between the particular phases [1, 2, 3] for the overall performance of the samples and its load-carrying capacity. An attempt to include the mechanical properties based on atomistic simulations is shown.

An analysis of samples of IPC based on SiC ceramic skeleton and an aluminum alloy under impact conditions is performed. The 3D structure of the sample is obtained with CT scans. The numerical model takes into account the properties of the interfaces between the phases. It has been noted that the interface properties are a significant feature of the materials and the resulting numerical model.

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A beam-like model for buckling and post-buckling analysis of a thin pipe

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Key Words: Thin pipe, beam-like model, buckling, postbuckling

Thin pipes are structural elements which are widely used in technical applications, especially concerning civil, industrial and aerospace engineering. The careful evaluation of their carrying capacity plays a key role in the design process, in particular due to the possible involvement of local effects related, for instance, to flattening or warping of the cross-sections. As a typical example, when pipes are bent over, the concurrent ovalization of the cross-section can induce a softening behavior, referred to as Brazier's effect [1], leading to a limit point in the bending moment-curvature relationship and a sudden failure of the structure.

Recently, a nonlinear beam-like model of thin pipe was proposed in [2, 3], where the classical kinematic descriptors for the rigid cross-section Timoshenko beams were combined to further descriptors, indicating amplitude of ovalization and warping under prescribed shapes. The obtained one-dimensional continuum model turned out to fully catch both nonlinear static and dynamic response of the pipe and, for its simplicity as compared to shell models, it appeared as very convenient to be tackled with perturbation methods.

In this paper, the above mentioned beam-like model is extended to address buckling and post-buckling analysis of thin pipes. For this scope, geometrical stiffness terms are consistently included and consequent evaluation of the critical loads is carried out. Numerical tools are then used to assess the post-buckling behavior, where the effect of cross-section change in shape can be prominent. Comparison with outcomes provided by finite element method commercial software, where the pipe is modelled as assembly of this shells, is carried out.

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A COMPUTATIONAL ANALYSIS FOR THE NONLINEAR MODEL OF A LAMINATED GLASS PLATE

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Key Words: *Glass, Plate, Composite, Finite Difference Method, Numerical Analysis, Nonlinear Modeling*

ABSTRACT

Laminated glass plates consist of two or more thin glass layers and an interlayer made of PVB (polyvinyl butyral). They can easily undergo large deflections since they are very thin therefore they need to be analyzed considering large deflection effects such as developing membrane forces etc. Consequently the equilibrium equations governing their behavior should be based on the large deflection theory.

Vallabhan et al. [1] modeled the laminated glass units and verified the mathematical model by comparing the results with the results of experiments conducted at the Glass Research and Testing Laboratory at Texas Tech University. Asik et al. [2] and Asik [3] made contributions by their research on the true behavior of glass units.

Four of the five equations are used to represent in-plane displacements in x and y directions and the last one for the transverse deflection of a unit. In order to obtain the governing differential equations, total potential energy of a unit is written as the summation of membrane, bending and force potential energies in terms of displacements.

The main difference of this study from previous ones is that employs free boundary conditions on two edges of the plates. For the other two ends the laminated unit is simply supported or fixed (clamped). Also the width of a unit which is not greater than the one-tenth of the length of a unit (which makes the unit a thin plate). Five coupled and partial differential equations obtained through variational principle for lateral and in-plane displacements. The governing differential equations are first discretized by finite difference method and then solved numerically by employing iterative solution procedures to obtain the displacements and stresses.

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Accurate and Efficient Quadrilateral Plate Element for Vibration Analysis of Laminated Composite Plates Using a Refined Third-Order Shear Laminated Plate Theory

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Key Words: *quadrilateral plate element, laminated composite plates, third-order shear deformation theory, quasi-conforming element technique, higher-mode natural frequencies*

An accurate, efficient and reliable four-noded quadrilateral plate element is developed in the present work for the vibration analysis of laminated composite plates. The element formulation is based on the quasi-conforming element technique (an assumed strain method) using a refined third-order shear deformation laminated plate theory proposed by the second author. The present quadrilateral plate element possesses higher accuracy than the conventional shear flexible plate elements, as it is derived from an assumed linear bending strain field. By using Hamilton's principle, the variational consistent equation of motion in matrix form corresponding to the third-order shear deformation theory is derived. The resulting mass matrices are decomposed into four parts: the usual part, the rotary inertia part similar to that in the first-order shear deformation theory, the part resulting from higher-order displacement and the part resulting from the coupling between the different components of the axial displacement. The higher-order and coupling mass matrices have a significant effect on the frequencies of high mode vibration. The element stiffness matrix and mass matrix of the present quadrilateral plate element are given explicitly and free from shear locking. Consequently, the present quadrilateral plate element is very computationally efficient. The average rotation across the plate cross-section is used in the refined third-order shear deformation laminated plate theory against the rotation at the plate mid-plane used in other higher-order plate theories, which leads to the correct boundary conditions to fix the rotation across the plate thickness. The free vibration examples of circular, square and skew composite plates are computed and discussed by using the present quadrilateral plate element. The effects of different boundary conditions, different aspect ratios and plate thickness are considered in this study. The numerical results show that the present plate element can give the correct results of the higher-mode natural frequencies. These numerical results clearly demonstrate that the quadrilateral laminated plate element presented in this paper is not only efficient but also very accurate.

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Auxetic metamaterial and flagstone tessellation patterns via convex Airy stress functions

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Key Words: *Graphic Statics, Flagstone tessellations, Auxetics, Metamaterials, Origami, Airy Stress Function*

This research paper presents a geometrical methodology for developing Auxetic metamaterials based on graphic statics. Specifically, it is shown how by employing reciprocal convex Airy stress functions [1] and Minkowski sums [2] it is possible to derive non-standard 2D Auxetic patterns with negative Poisson's ratio. Furthermore, it is discussed how said geometrical construction underpins origami flagstone tessellations [3].

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Design Optimization of a Single-Phase Elastic Metamaterial for Enhancing Mechanical Resistance to Impact Load

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Key Words: Design Optimization, Single-phase Metamaterial, Stress minimization, Impact load

Elastic metamaterials (EMMs), which are architected materials with unique properties due to the presence of bandgaps – frequency ranges in which the wave propagation is attenuated – have drawn attention of researchers to their effectiveness in attenuating waves. Unlike phononic crystals (PnCs), which are periodic structures that exhibit bandgaps due to Bragg scattering, EMMs rely on the use of internal resonators [1]. This type of locally resonant structures have shown promising results for attenuating low-frequency waves as the ones originating from repetitive impact loads [2].

The use of single-phase EMMs has recently been investigated, because their manufacturing requires less complex and low-cost processes. Furthermore, with the trend of circular economy, such EMMs can be manufactured from raw disposal materials or can be easily re-processed for other applications. However, obtaining a low-frequency bandgap by using such single-phase structures requires large masses and thin structures targeting low stiffness, which may result in impractical designs from a mechanical point of view. In order to overcome such limitation, optimization techniques can be used to enhance the mechanical properties of the unit cell by minimizing the stress.

This work investigates the mechanical behavior of a single-phase EMM formed by a cylindrical inclusion connected to the frame by four beams. The aim is to filter energy at specific frequencies of an impact signal. The unit cell shows bandgaps at a low frequencies, which are related to the geometric parameters of the internal resonator. It is observed that the EMM fails mechanically due to high-amplitude loads, especially because of the requirement of thin beams and huge masses to obtain low-frequency bandgaps. The proposed scheme optimizes the geometric parameters so that the stresses are minimal, while keeping the bandgap unaltered. Through such procedure, the metamaterial can be used for vibration suppression and noise control of structures undergoing high amplitude impact loads.

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Homogenized Model for Masonry Walls Retrofitted by Steel Fibre reinforced Mortar Coating

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Key Words: *Retrofitted masonry; Homogenization; Linear elasticity; Static and dynamic analyses.*

The unreinforced masonry has been used for constructing a large number of buildings placed in seismic areas worldwide. It is well known that the typical low tensile strength of this material makes existing buildings vulnerable to both in-plane and out-of-plane seismic actions. For this reason, a lot of research studies are devoted to develop and improve retrofitting techniques for enhancing the seismic behaviour of masonry buildings. Among these, an innovative technique that combines the advantages of traditional methods with the use of advanced materials is represented by Steel Fibre Reinforced Mortar (SFRM) coating. This rather new retrofitting method consists of a thin mortar coating, bonded either on one or both sides of masonry elements and reinforced with short fibres. The literature about this topic regards mainly experimental tests (see [1-3]). On the other hand, the specific modelling of SFRM and of its interaction with masonry structures is rather lacking.

In this work, the idea is to replace the fine model of the wall retrofitted by SFRM with an 'equivalent' homogeneous Mindlin–Reissner plate, having unitary thickness and the same stiffness and mass of the nonhomogeneous model. A homogenization procedure is applied to an elementary cell to derive closed-form expressions for the linear elastic constants of bending and twist stiffness, of the out-of-plane shear stiffness and of the membrane stiffness. The stresses of the masonry and SFRM components are also evaluated analytically once the average stress acting on the homogeneous medium is determined. Parametric analyses are carried out to evaluate the influence of the reinforcement system on the equivalent material properties, by varying the thickness and the elastic properties of the SFRM. The accuracy of the theoretical results is assessed by means of comparisons with finite element (FE). Finally, static and dynamic FE analyses are carried out on sample masonry walls, with the aim of comparing the non-homogeneous and homogeneous models. The mechanical performances of the structures are investigated according to the effectiveness of the SFRM.

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Nonlinear electro-mechanical dynamics of a piezo-composite beam rotor system

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Key Words: active composite beam, piezoceramic material, rotor, nonlinear constitutive behaviour

A system consisting of the active composite beam clamped to the rotating hub is considered. A combined shearwise bending and twist deformation of the blade as resulting from directional properties of a composite substrate (core) is considered and relevant kinematic relations are formulated within geometrically linear framework [1]. To match the experimental results published in literature [2] and to enhance the generality of the proposed formulation a nonlinear constitutive behaviour of the piezoceramic material layer is assumed. Finally, nonlinear inertia effects related to the system rotation are taken into account.

The mathematical model of the system is formulated by means of the extended Hamilton's principle. Since the piezoceramic layers exhibit nonlinear material properties the relevant component of the potential energy is calculated as a volumetric integral of the electric enthalpy density function. The derived system of three integro-partial differential equations represents the electro-mechanical behaviour of the system. In particular, the beam dynamics is represented by a generalized displacement coordinate and an output voltage coordinate; the behaviour of the rigid hub is given by its rotation angle coordinate. The state equations are discretized by the Galerkin's method and next solved around the first resonance zone for the system excited by periodic torque supplied to the hub. The obtained response curves reveal strong softening behaviour resulting from nonlinear constitutive properties of the active piezoceramics. Moreover, additional unstable solutions have been identified out of the resonance zones. It's observed the magnitude of the softening effect and width of unstable zones decreases while the mean rotor angular velocity is increased.

A series of further numerical simulations is performed to examine the impact of torque excitation amplitude, torque mean value, hub inertia and electrical load resistance on system behaviour. Next, the performance of the system with parallel or in-series connected transducers is discussed and both configurations are compared in terms of energy harvesting efficiency. Finally, the impact of composite reinforcing fibres orientation/laminate configuration represented by various bending/torsional coupling ratios on system dynamics is studied.

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On the effects of different types of nonlinearities in fast/slow dynamics of a meta-cell

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Key Words: meta-cell, compound nonlinear restoring force, slow invariant manifold, fast/slow dynamics

Metamaterials are systems designed to exhibit some properties which can not be found in nature [1]. One special type of metamaterials is the mass-in-mass system, which can present interesting properties such as equivalent negative mass and stiffness. The studied system, a mass-in-mass unit cell, possesses a nonlinear restoring forcing term, $F(\alpha)$, which depends on the relative displacement of the two masses m_1 and m_2. In this work, several types of nonlinearities (unique and compound), presenting smooth or nonsmooth restoring forcing functions, are considered. System variables are complexified [2] and the resulting dynamics is treated via a time multiple scale method. It will be shown that systems with compound nonlinearity may present some characteristics which differ from systems with classical nonlinearities. Moreover, the frequency responses of the system can present isola, which should be taken into account carefully for control aspects.

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Prediction of Thermal Buckling Temperature of Sandwich Plates with Lattice Core

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Key Words: *Lattice, Sandwich Panels, Thermal Buckling, Critical Buckling Temperature, Global and Local Buckling, FEM*

In recent years, the development of spacecraft for re-entry into the atmosphere has been revived due to the acceleration of private-sector space development. During re-entry, the spacecraft is subjected to an extremely high thermal load, which may lead to thermal buckling of the spacecraft. It is important to correctly estimate the buckling temperature of mechanical structures that are subjected to thermal loads, because this phenomenon can lead to serious accidents due to performance degradation and damage.

Over the decades, many studies [1, 2] have been reported on the thermal buckling of flat plates, composite plates, and sandwich structures, which are commonly used in airframe structures. For example, Chen et al. derived a theoretical equation for the critical buckling temperature of a lattice sandwich panel with a pyramidal core in the deformation mode where the panel buckles as a whole, with the core homogenized [3]. However, the buckling behaviour depends on not only the macroscopic mechanical properties but also the micro-architecture of the panel, so it is inadequate to estimate the buckling temperature from the homogenization method only.

In this study, the finite element analysis was conducted on the composite panel with lattice core by modelling the exact micro-architecture. In particular, the effects of geometric properties such as core height, core length, and number of cells were investigated. As a result, it was confirmed that there are mainly two types of thermal buckling modes for sandwich panels: global and local buckling modes, and that the global buckling mode is affected by the number of cells in the panel. The global buckling temperature can be estimated with good accuracy by multiplying the analytical equation derived from the conventional homogenization method by a correction factor including the effect of the number of cells. On the other hand, the local buckling temperature can be estimated by considering the buckling behaviour of a small plate surrounded by the cells and supported by four corners. The analytical equations for the global and local buckling temperatures presented in this study can be used to quantify the design of lattice sandwich panels.

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RESPONSES OF A NON-LINEAR PERIODIC MASS-IN-MASS CHAIN DURING A SINGLE MODE EXCITATION

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Key Words: non-linear meta-materials, mass-in-mass cells, fast/slow dynamics

Meta-materials are developed to present unusual non natural responses against external or internal actions. In the vibro-acoustics domain, mass-in-mass systems are one type of meta-materials which are developed for vibro-acoustic applications. For this purpose, the following L-periodic chain is composed of non linear cubic mass-in-mass cells which are coupled linearly. Forcing is applied on the whole chain with spatial sinusoidal weighting derived from the dispersion equation.
The discrete form of system equations is transferred to continuous domain. Then, the study is conducted using multiple scale methods [1] in order to analytically determine the dynamical behaviors of the chain. The dispersion equation is obtained by considering the linearized associated system. Complex variable of Manevitch are introduced to simplify the understanding of fast and slow system dynamics [2]. Fast dynamics leads to detection of the slow invariant manifold and its stable zones. Slow dynamics leads to detection of singular and equilibrium points, allowing to establish bifurcation points and the frequency responses. The analytical work is verified by numerical simulations on the discrete periodic initial chain. For each cell, its seen that equilibrium points, as functions of deriving frequency, can be located in the main branch of the frequency response or on isola, either in stable or unstable zone of the slow invariant manifold. Moreover, depending on the property of the point, the system can present periodic or non-periodic responses. The development provides necessary tools for designing such a chain for localization of the vibratory energy inside some zones of a targeted mode.

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Spectral design and nonlinear dispersion properties of a mechanical metamaterial with local inertia amplifiers

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Key Words: Pantographic Metamaterials, Wave Propagation, Spectral Design, Nonlinear Dynamics

Architected metamaterials yielding superior dynamic performances can be conceived by realizing local mechanisms of inertia amplification in the periodic microstructure [1]. A periodic cellular waveguide characterized by an intracellular pantograph mechanism is considered as minimal physical system simulating an inertially amplified metamaterial [2]. A discrete tetra-atomic model is formulated to describe the undamped free dynamics of the cell microstructure. The ensuing ordinary differential equations of motion feature quadratic and cubic inertial nonlinearities, induced by the axial indeformability of the pantograph arms connecting the principal massive atoms with the secondary massive atoms, serving as inertial amplifiers. First, the linearized model is investigated to analytically design the metamaterial spectral properties. To this aim, the band structure of the complex-valued dispersion spectrum is determined analytically, and a spectral design problem is stated and solved by inverting the functions expressing parametrically the boundaries separating attenuation (stop) and propagation (pass) bands in the frequency spectrum. Upon demonstrating the existence of feasible design solutions, the analysis provides complete definition of the physically realizable band structures in the frequency domain and alternative criteria to design iso-band structured metamaterials [3]. Moving to the nonlinear model, dispersion properties governing the free undamped propagation of harmonic Bloch waves are investigated in absence of internal resonances. The multiple scale method up to the third order is adopted to analytically determine the nonlinear functions relating dispersion properties and oscillation amplitude of the propagating acoustic and optical waves. Specifically, the nonlinear wavefrequencies and waveforms are determined as analytical closed-form functions of the parameters, quadratically depending on the oscillation amplitudes. Validation of the analytical outcomes, performed by directly integrating the nonlinear equations of wave motion for different initial conditions, confirms the goodness of the asymptotic approach.

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VIBRATORY ENERGY CHANNELLING BETWEEN A LINEAR AND A TIME-DEPENDENT NONLINEAR OSCILLATOR

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Key Words: Targeted energy transfer, time-dependent nonlinear rigidity, control, meta-cell

We consider a system composed of a linear oscillator which is linearly coupled to a nonlinear oscillator with a time-dependent nonlinear stiffness. We study the energy exchange between two oscillators for vibration control [1]. For this we detect the fast and slow dynamics of the system [2] in order to find out its fixed points and different possible regimes, i.e. periodic or non periodic ones [3]. Thus, the behaviour of the system can be predict. This study permits to reveal the Slow Invariant Manifold (SIM) of the system and its singular and equilibrium points. We spot that the geometry of the SIM of the system with variable rigidity is different from the one with constant nonlinear rigidity. The non classical geometry of the SIM and atypical positioning of system singularities (ranging from continuous to closed form curves on the SIM depending on the system parameters) creates energy channelling between two particles which depend on the phase of the system. Our developments permit to design the energy channelling (and so tunning system parameters) between two oscillators (or particles). The system under studying can be seen as a time dependent nonlinear "meta-cell".

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Compliant Folding Hinge Structure using Radial Slit Pattern

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Key Words: *Origami, Thick Origami, Compliant Mechanism, Hinge, Slit Pattern*

Origami models are often idealized by discrete folding of zero-thickness sheets; however, the sheet thickness and the elastic limit of the material cannot be ignored in engineering practice. Existing studies realize the folding deformation of origami structures in the elastic range of the material by replacing the crease lines with a wide deformation zone with slit patterns on it [1, 2]. However, this approach based on a compliant hinge has several limitations. Namely, the wide hinge cannot maintain the center of rotation between panels during the folding motion, so it is difficult to accurately deploy the origami structure with interior vertices where multiple crease lines meet. In addition, the play caused by the width of the deformation zone increases the degree of freedom of the origami structure, leading to the instability of the folded structure.

To solve these issues, we design a new hinge structure based on composing parallelly connected compliant spherical joints through the use of the theory of flexure joints [3, 4]. Specifically, we create a spherical joint by radially placing the Lamina Emergent Torsion (LET) joint [5, 6]. Then, we arrange multiple spherical joints in a straight line to create a fixed axis, which acts as the hinge.

The proposed hinge structure is evaluated through an experiment and simulation. The experiments show that the center of rotation is maintained up to a wider range of fold angles when compared to the general LET joint. Then, we verified that the shape of the hinges in the experiment and the simulation match well. By conducting optimization based on the genetic algorithm in the simulation model, we obtained patterns that minimize the maximal curvature of the hinge.

Since the proposed hinge structures can be manufactured from a single plate material through 2-axis CNC cutting or laser cutting, the whole origami structures using the hinge can also be manufactured from a single plate. Potential application of this hinge structure includes kinematic facade, foldable displays, and deployable solar panels.

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Experiment of a Semi-Active Electromagnetic Seismic Isolation System

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Key Words: *Electromagnetic damper, Semi-active Control, Shaking Table Test.*

A near-fault (NF) ground motion can induce considerable base displacement and structural acceleration in a seismic isolation system. In order to improve this problem, adding viscous dampers in isolated systems in NF regions has been recommended by researchers. However, a high damping ratio can induce high structural acceleration of a seismic isolation system when subject to far-field ground motions.

In this study, a novel semi-active electromagnetic seismic isolation system (SA-EMSIS) was developed. The SA-EMSIS consists of a passive EMSIS [1] and an electrical resistance controllable module. The EMSIS is composed of an EM damper, sliding platform, and a pair of springs. The EM damper is composed of a DC motor, gearbox, and rack and pinon mechanism. The semi-active control algorithm can be achieved by adjusting the external resistance of the circuit in real time via the resistance control module. By combining the seismic early warning technology in the future, the SA-EMSIS can perform adaptive EM damping coefficient under different types of excitations. In this stage, a prototype of the SA-EMSIS was designed and manufactured. The relationship between the equivalent EM damping ratio and the corresponding total electrical resistance of the circuit was identified via sine-sweep test. Semi-active control algorithms were also tested to investigate the controllability of the electrical resistance controllable module.

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Flattening Response of Net-shaped Circular Tubes Under Pure Bending

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Key Words: Mechanical Properties, Structural Analysis, Flattering, Pure bending, FEM

A net-shaped structure is recognized as a component of truss structure and a lot of researches have been reported. For example, there are lightweight roof structures in structural engineering and cylindrical structures such as stents and McKibben actuator in the mechanical field.

On the other hand, the cross-sectional flattening in pure bending of cylinders has been investigated by many researchers[1, 2, 3, 4]. The circular tubes have also been used in many kinds of machines and structures as a structural part.

According to their previous studies, it is found that there are mainly two factors that dominate the collapse of cylinders subjected pure bending loading. Chen has investigated the elastoplastic pure bending collapse of cylindrical tubes using the non-linear finite element analysis. In his study, the flattening velocity parameter v_b is introduced to evaluate the flattening response of tubes. Also, based on his numerical investigation, he proposes a theoretical model for predicting the bending moment-curvature relationship.

In this paper, the elastic bending collapse of net-shaped circular tubes subjected to statically pure bending is studied by using finite element method (FEM). Comparison with equivalent shell structures, net-shaped circular tubes are more flexible and slow down the bending collapse. In net-shaped circular tubes, the slope of the flat line is $v_b = 2$, but the intercept is different depending on the density. Thus,increasing the density, the flat line brings near to the shell's. From the proposed flat line, it is possible to predict the response of the bending moment to bending curvature regardless of the micro-architecture of the net.

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Harnessing Bistability of Domes using Piezoelectric Actuation to achieve Patterned Sheet Structure with Adaptive Mechanical Properties and Shape

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Key Words: Bistability, Piezoelectric actuation, Shape-morphing, Adaptive structures

For decades, numerous efforts have been made to design structures against buckling and instabilities, which often lead to their catastrophic failure. By contrast, recent studies have shown that harnessing mechanical instabilities can provide structures with new features as negative stiffness and energy dissipation [1]. Domes are shell structures that can exhibit up to two stable states, mostly depending on geometric and material parameters [2]. Apart from its basis state, a dome can be subjected to snap-through buckling and remain stable in this state indefinitely over time in absence of external loadings, being then considered as bistable. Recently, studies showed that bistability of domes may be used for shape morphing of sheets [3] and mechanical programmability [4].
The present work exploits snap-through buckling in dome-patterned structures to design novel responsive surfaces whereby the local topography is triggered by bistability and is reversed using an external electric field. The mechanical dome-like systems are designed with the help of finite element (FE) simulations, and are then realized via 3D printing for testing under electro-mechanical loading.

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Heat Transfer Characteristics of BCC lattice Core on the Heated Plate Under Impinging Flow

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Key Words: *Heat transfer, Pressure drop, Porous structure, Finite element method*

Over the decades, due to the rapid development of engineering, a large number of high-load electronic devices have been developed, and rapid the increase in processing speed and computational load has led to a high heat generation density. To remove heat from the equipment efficiently, many kinds of cooling devices such as have been proposed. One of the candidates of the cooling device is equipped with air impinging jets. Many studies on the heat transfer characteristics of air impinging jets using flat surfaces have been conducted by many researchers [1]. On the other hand, heat transfer characteristics using porous materials have also been actively studied in recent years due to their ability to provide a large surface area even in a low volume, and their application to heat sinks with various cooling methods has been investigated[2].
Recently, the development of laser processing technology has led to the rapid spread of metal 3D printers, which are expected to be applied in various fields as they are capable of modeling structures with fine and complex shapes with diameters of several hundred micrometers. The lattice structure with the length of micrometres can be fabricated by a 3D printer, and is expected to make it easier to predict the heat transfer characteristics.
The number of reports on heat transfer experiments using heat sinks formed by 3D printers is gradually increasing[3], but there are few verification examples of the application to jet flow models.
In this study, a BCC structure is selected for investigation, and its heat transferring response of the BCC heat sink were investigated using the finite element method. Here, the BCC lattice is located on a heating block, and coolant air is blowing from the top surface through the impinging jet. In particular, the effects of fin height and heat transfer characteristics on the heat sink with BCC structure were also investigated. It was confirmed that the heat sink with BCC structure can possesses superior heat conduction and heat transferring capacity to the coolant under the slower flow speed.

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Investigations on novel active tristable cross-shaped laminates

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Key Words: *Tristability, Composite, Cross-Shape, MFC Actuators, Snap-through*

Morphing multistable structures are highly attractive for advanced shape-changing applications due to their low weights, excellent mechanical properties, and large deformation capabilities. Multistable composite structures have at least two stable configurations; each configuration represents a different geometry and can withstand significant changes in its shape without a continuous power supply [1]. Aim of the paper is to develop a tristable cross-shaped structure, consisting of unsymmetric laminates actuated using Macro Fibre Composite (MFC) actuators. With the advancements in flexible piezoelectric materials, actuation with MFC actuators is proved as a faster and efficient method to change the shapes of multistable laminates [2]. The cross-shaped tristable laminates find potential applications in solar tracking models and energy harvesters. The critical snap-through voltages required to change the shapes are investigated using commercially available finite element package. Use of planar MFC actuators to snap the bistable laminate from one equilibrium shape to another is demonstrated. MFC actuators are bonded on both sides of the four legs to trigger multiple snap-through events. The third stable equilibrium configuration is a transition state which occurs in the snap process from the first to second equilibrium configurations. The snap processes, including the first–third–second and second–third–first, between the different stable equilibrium configurations of tristable cross-shaped unsymmetric laminates are investigated. An attempt is made to address the possible design difficulties arising from the additional stiffness contribution by MFC layers on the naturally cured equilibrium shapes of cross-shaped tristable laminates. Suitable potential applications using the designed self-resetting active tristable cross-shaped laminate are proposed.

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Kinematics of an Origami Inspired Millipede Robot

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Key Words: *Origami, Bioinspired, Kinematic Analysis, Spatial Linkages, Robotics*

Worm-like robots have received great attention due to their ability to navigate through limited space and crawl over uneven surfaces. The living organisms like earthworms, usually consist of several continuous body segments to achieve peristaltic movements [1]. To mimic such behaviours, roboticists have adopted various approaches to design versatile worm-like robots. For instance, soft materials have been used to achieve radial and longitudinal expansion on body segments, and thus a retrograde peristaltic wave is produced [2]. Origami also offers a simplified way to design metameric segmentation capable of locomotion through length variation and body rotation [3].

While resembling worms in many ways, a millipede is not a worm but an arthropod whose body segments are covered by stiff outer skins. When sensing danger, it curls into a spiral, which is a self-defensive mechanism and protects it against predators [4]. Inspired by this specific organism, our research is to develop an origami-based concept for a robot that replicates peristaltic and curling motions similar to those of a millipede.

The proposed mechanism is made with a chain of interlinked modules, mimicking the segments in a millipede. In contrast with the usual origami approach where zero-thickness sheet materials are used, our module is an assembly of deformation free facets with uniform and finite thickness, connected along their upper or lower edges by creases and thus forming an origami pattern of thick panels. Kinematically, a module includes two types of Bricard linkages. Since it has been known that the finite thicknesses of origami facets can reduce the overall degrees of freedom (DoF) [5], our module has only one DoF with kinematic bifurcations. Moreover, the module is specially designed so any numbers of modules can be linked while the single mobility feature is preserved.

This works focuses on the kinematic aspect of a millipede robot. A detailed analysis of the origami mechanism is to be presented, where the curling and peristaltic motions are quantified kinematically. The motion paths are given, with bifurcation configurations identified for motion switch. In addition to the two typical millipede movements, three more configurations of the origami, i.e., a wave, a bench, and a heart, are displayed, bringing the potential for locomotion mode change and opening up additional design space with targeted applications. Our concept is validated by both kinematic simulations and physical models. The work paves way for the realisation of millipede-like robots in the future with actuation and control components integrated.

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Mechanics of Morphable Architected Materials

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Key Words: *Origami, Kirigami, Morphing, Reconfigurability, Temperature Stimulus*

Materials capable of transforming their shape in response to an external stimulus hold promise for application in multiple sectors, from aerospace, robotics, to mechanical and civil engineering. In this talk, I will present a set of reconfigurable metamaterials developed in my group that leverage their mechanics to morph in response to either an applied force or to a change in environmental temperature. On the first front, I will present a class of reprogrammable cellular origami that can not only rigidly fold but also lock into several stiff states that are load bearing in multiple directions. On the second front, I will show examples of temperature-induced morphing, such as a multimaterial truss that can reversibly adapt its structure without forgoing structural capacity, and a class of transformable smart metamaterials that undergo topological changes and giant thermal expansion.

Multi-stable structures induced by pneumatically inflated pouches with laid-in origami paper pattern

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Key Words: *Instructions, Multiphysics Problems, Industrial Applications, Covid-19*

When a surface bounded by an inextensible frame shrinks, it buckles and forms a saddle shape. Such a surface can be realized by pleating a sheet of paper [1] or by pre-stretching membrane and attaching it to a 3D printed frame [2]. In particular, the system provides a multi-stable structure when the boundary frame is polygonal [1].

Inspired by the concept of pouch motors [3], we introduce a novel method for providing multi-stable surfaces by pneumatically inflating these surfaces along the patterned frame. We fabricate the structure from two layers of nylon film with heat adhesive layers and the patterned sheets of paper in between. When the structure is heated, the films fuse except for the paper covered part which forms a pouch of desired pattern. We show how the inflation of pouches induces multi-stability by comparing it with prestressed membranes and origami systems.

We applied various geometric patterns inspired by origami to our pouch-based system to produce switchable surfaces. We also show the behaviors of cellular structures obtained by stacking such surface structures.

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Origami Metamaterials with Near-Constant Poisson Functions Over Finite Strains

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Key Words: *Origami, Metamaterials, Mechanics, Large deformation, Poisson's ratio*

Origami-based structures have gained interest in recent years due to their potential to develop lattice materials, called metamaterials, whose mechanics are primarily driven by the unit cell geometry. The folding deformations of typical origami metamaterials result in stretch-dependent Poisson's ratio, and therefore in a Poisson function with significant variability across finite deformation. This limits their applicability as the desired response is retained only for a narrow strain range. To overcome this limitation, a class of composite origami metamaterials that exhibit nearly a constant Poisson function, specifically in the range of -0.5 to 1.2 over a finite stretch of up to 3.0 with a minimum of 1.1, is presented. Drawing idea from the recently proposed Morph pattern, the composite system is built as a compatible combination of two sets of cells exhibiting contrasting Poisson effects. The number and dimensions of the cells are optimized for a stretch-independent Poisson function. The effects of various strain measures in defining the Poisson function are also discussed. The results from the study are validated using a bar-and-hinge-based numerical framework capable of simulating the finite deformation behavior of the proposed designs.

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Sound Absorption in Semi-Closed Cellular Structures Fabricated by 3D Printer

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Key Words: *Sound absorption, Porous structure, Homogenization method, 3D printer*

In recent years, due to environmental regulations and industrial development, there has been a growing interest in noise problems and their reduction, and the demand for components used for soundproofing has increased. Currently, porous materials such as glass wool and urethane are widely used, and research on foam materials using metallic materials has already been conducted [1].

In general, in order to improve the sound absorption performance of porous materials, we can make the pores inside the material as small as possible and increase the tortuosity of the air passing through the pores to dissipate the acoustic energy as heat loss.

On the other hand, the rapid development of laser processing technology in recent years has led to the widespread use of powder metal 3D printers, and their active use in manufacturing has been increasing. Since metal 3D printers directly use CAD data for manufacturing, it is relatively easy to fabricate micro-lattice structures consisting of minute beams with diameters of several hundred micrometers.

One of our co-authors [2] investigated the sound absorption characteristics of a lattice structure that can be fabricated by a powder-bed metal 3D printer by numerical analysis and sound absorption experiments using acoustic tubes. The structure is composed of body cantered cubic (BCC) structure with partially closed surface which can be manufactured by the printer. The numerical analysis is based on the homogenization method which takes into account the multiphysics occurring in poroelastic media including elastic deformation in the solid phase, compressive viscous fluid flow and the pressure and temperature distribution in the fluid phase, which has already proposed by Yamamoto et al. [3].

In this study, the sound absorption capacities of another type of porous structure with partially closed walls have been investigated by using the same numerical approach. The structure is based on the octahedral lattice cell with partially closed surface, and has great potential to absorb sound sufficiently as well as possessing high structural stiffness. Based on the numerical analysis, the effects of micro-architecture on the sound absorption capacity as well as the contribution of the dissipated energy are discussed.

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Two-dimensional analytical solution for multi-segmented Al/ steel-composite panel-An Aerospace Application

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Key Words: *composites, 2D exact, panel, dissimilar material*

Abstract:

E-vehicles and light weight structural parts in automotive and aerospace industry has led to design and development of new structures where traditional materials aluminium/steel are joined with composite laminated materials. This approach has led the engineers/researchers to reduce weight and ultimately save fuel consumption and reduce carbon footprints.
Moreover, prosthetic limbs are also designed to have varying material along the length for better suitability. The above problems cannot be analysed using functionally graded theories/concepts. In theory, material properties vary linearly, exponentially, or power-law-like along x-values but for the above cases, material property does not follow a particular variation. Further even, it is not always practical to produce or manufacture components having very smooth variations along the length.
Number of research articles are reported on the development of joining techniques for the dissimilar materials [1,2]. Bending, free vibration and buckling analysis is also needed for theses case [3]. At the joining or interface point, local inplane and transverse stresses may rise sharply and may cause debonding and failure of structures. One dimensional analysis based on classical assumption or higher order can not accurately predict the stress behaviour at theses places.
In this paper, an attempt is made to develop the 2D analytical solution for multi-segmented Al/ steel- composite panel under transverse loading. Extended Kantorovich method is used for developing governing equations. Continuity of displacement and stresses are satisfied at interface of each segment. Two segmented panels having aluminium/steel and Gr/Ep equal and unequal segment are considered. The deflection and stresses are compared with the finite element solution and found in good agreement.

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Anti-plane wave scattering of anisotropic elastic materials using the MFS

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Key Words: Anti-plane wave, Anisotropy, The method of fundamental solutions

In recent years, anisotropic materials such as fiber-reinforced plastics (FRP) have been increasingly applied to civil engineering structures. Anisotropic materials have different mechanical properties depending on the direction, and wave propagation in anisotropic materials is known to be more complicated than that in isotropic materials [1]. Therefore, numerical simulation of wave propagation and scattering in anisotropic elastic materials play an important role in not only understanding their characteristics but also developing nondestructive evaluation techniques.

The method of fundamental solutions (MFS) is a numerical technique of mesh-free type for solving partial differential equations [2]. The MFS uses fundamental solutions as a basis function, and the source points of the fundamental solutions are located in the complementary domain of analysis one. The MFS requires fewer unknowns than the finite difference method (FDM) and the finite element method (FEM), because it does not require mesh generation of domains and boundaries. In addition, numerical implementation of the MFS is easier than that of the boundary element method (BEM), because the MFS can avoid the singular integration over the boundary. On the other hand, there are few applications of the MFS to wave problems in anisotropic elastic materials.

In this study, we apply the MFS to anti-plane wave scattering of anisotropic elastic materials. Numerical results computed by the proposed MFS are compared with those of the conventional BEM for the validation of the proposed method. Afterwards, we discuss the relationship between the source point location and computational accuracy.

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Deep-learning based inverse scattering for a defect in 2-D isotropic solids

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Key Words: Time-domain BEM, Deep learning, Inverse scattering, Ultrasonic non-destructive evaluation, Defect shape reconstruction

The inverse scattering analysis that reconstructs the defect shape using the scattered waveforms from a defect obtained by an ultrasonic array transducer has been performed for a long time. In general, the inverse scattering techniques based on the Born, Kirchhoff approximations [1], and time-reversal approach are known as relatively time consuming methods. On the other hand, the machine-learning is attracting a lot of attention in many engineering fields. In particular, the deep learning (CNN: Convolutional Neural Network), which is an extension of the neural network (NN), has become a basic technology for creating an artificial intelligence (AI). In the field of the ultrasonic nondestructive evaluation (UT), the inspectors have to make a judgement whether test materials have a defect or not using scattered waveforms from a defect. This operation requires a great deal of skill of UT inspectors and the UT accuracy depends on the inspector skill.

To overcome this difficulty, in this study, a deep learning is utilized to detect a defect in 2-D isotropic solids. The images required for the present deep-learning with the convolutional neural network (CNN) are numerically prepared using the convolution quadrature time-domain boundary element method (CQBEM) [2] for simplicity. The CQBEM is known as a suitable numerical approach for wave analysis and can produce high precision solutions better than the classical time-domain boundary element method (BEM). In the CQBEM analysis, scattered waveforms by a defect at some receiver points are artificially produced. These waveforms as a function of the time are transformed into the color mapped image data. These color mapped image data are given for input data as the CNN. As numerical examples, some defect position and scale detection problems are solved by using the created deep learning model. The results for how the created deep learning model determines the defect position and scale may be useful for future practical application of this method.

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Detection of Bi-Material Plate Debonding by Guided SH Waves Scattering with BEM

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Key Words: *Guided SH waves, Scattering, Debonding, Boundary Element Method*

This research aims to investigate the guided shear horizontal (SH) waves scattering phenomena used in the non-destructive inspection for detection of interface debonding in bi-material plate structures. A boundary element method (BEM) is used to solve the scattering problem of SH guided waves due to efficiently and accurately in computation, leading to the reflection and transmission coefficients of scattered waves. Two-dimensional, isotropic, linearly elastic, and traction-free plate structures are considered. This plate is a perfectly bonded bi-material that is split between upper and lower layers. The interface containes a finite length traction-free debonding which acts as a scatterer for propagated guided waves. The frequency domain, elastodynamic fundamental solutions of traction and displacement are utilized for boundary integral equations. Wave functions are formulated by the partial waves technique to obtain the dispersion curves and wave structures. Discretizing boundaries surrounding bi-material plate domains into constant elements yields a system of linear equations, which can be solved by a regular linear solver. Various parameters in numerical calculation are considered including materials, debonding lengths and locations with selected modes of an incident wave over several frequency ranges. Obtained results show the scattered guided SH waves have the potential to detect a debonding. Bi-material structures also affect the uncouple of symmetric and antisymmetric properties leading to the mode-conversion phenomena. Moreover, the resonance phenomena can also be observed where all the waveforms are reflected and cannot pass through the debonding. Such information will establish fundamental knowledge for non-destructive inspection and structural health monitoring.

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Inverse Analysis of Wave Sources Based on Sparse Estimation

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Key Words: Inversion, Wave Source Imaging, Anti-plane Wave, Sparse estimation, LASSO

Recently, ultrasonic flaw imaging has become popular with the development of a multi-point measurement system such as a phased array method. Particularly, FMC/TFM (Full Matrix Capture / Total Focusing Method)[1] is a powerful post-processing tool to produce the best flaw image at each focusing point. In FMC/TFM, however, lots of data have to be handled, which are collected from each transmitter/receiver combination. Therefore, an effective inversion approach for flaw imaging using less data is expected. In this paper, an innovative wave inversion based on sparse estimation is investigated by numerical simulation.

The problem is to estimate an anti-plane wave source from waves observed at several points surrounding the source. The wave source is approximated as an equivalent body force, and the radiated waves are formulated in a simple integral form, which gives the relation between the radiated waves at observation points and the source parameters. Unfortunately, the discretized integral equation with unknown source parameters becomes ill-conditioned. To overcome this difficulty, the LASSO[2] approach is applied to solve the discretized integral equation on the assumption that the source parameters are distributed sparsely in the domain.

In numerical simulation, first, the anti-plane waves radiated by the given source are numerically calculated at the observation points. Then the location and strength of the equivalent body force are determined from the simulated wave field using LASSO. The applicability of the sparse estimation is demonstrated by several simple numerical examples.

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Numerical Continuation and Semi-analytical Finite Element Method for Guided Wave Dispersion Analysis

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Key Words: Guided Wave, Finite Element Method, Continuation Method, Dispersion Curve

In the non-destructive testing (NDT) and structural health monitoring (SHM), it is required to know dispersion relations to better understand a propagating wave in an elongated material. To analyze the dispersion phenomenon in terms of frequency and wavenumber, analytical approaches have been applied for elongated structures with simple-shaped cross-sections. On the other hand, numerical approaches are often used to calculate the dispersion curves for a waveguide with an arbitrary cross-section. Although several numerical methods have been proposed for the dispersion analysis in conventional researches, we focus on a semi-analytical finite element method [1] (SAFE) herein.

In the SAFE formulation, the target domain is discretized in the cross-section, while an analytical solution is adopted in the wave propagation direction. Then, the eigenvalue problem is constructed in a similar way to general finite element methods. The dispersion relation can be obtained to solve the eigenvalue problem for the wavenumber by sweeping the frequency. However, the dispersion curve becomes tangled for materials that have a complicated cross-section and an inhomogeneity. In particular, it is known that the dispersion curves for composite materials often exhibit an acute directional change. Thus, it sometimes would be difficult to classify each modal curve and to evaluate the continuity of the curve.

This study proposes a mode tracking method of the dispersion curves using a numerical continuation method [2] (NCM). In the proposed method, nonlinear algebraic equations are formulated from the eigenvalue equation provided by the conventional SAFE. Since the dispersion curves are smooth even in the discretized system, the NCM can track the dispersion curve continuously based on the Newton-type iteration method. To prevent a jump from a dispersion curve to other ones in the tracking process, we introduce several constraints.

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Time evolution of multiple scattering of point-like scatteres based on a Volterra type integral equation

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Key Words: Time evolution, Multiple scattering, Point-like scatteres, Volterra type integral equation, Krylov subspace method, FFT

Concept of point-like scatterers is as a result of the mathematical idealization for cases that the spatial scale of the scatterers are very small compared to the wavelength of the back ground structure of the wavefield. Applications of point-like scatterers for scattering problems spreads to wide range of analyses such as crystallite granite. This study develops a method for a time evolution analysis of multiple scattering problem of point-like scatterers and investigates the properties of interaction effects in the time domain based on the numerical computations. The method employs the Volterra type integral equation with respect to the time evolution. The formulation itself is based on previous studies in the frequency domain (e.g. Foldy [1], Waterman and Truell [2], and Hu and Sini [3]). The fast Fourier transform and Krylov subspace method are employed for the analysis of the Volterra type integral equation, in which the kernel of the integral equation is derived from the Foldy model[1]. Numerical computations are carried out for one configuration model. Numerical results showed that time evolution of the scattered wave field is well explained by the retarded time as well as the geometrical attenuation of waves from each scatterer. Incorporation of statistical as well as renormalization approach to the present model is the task for the future.

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Modelling local energy dissipation mechanisms in the seismic response of reinforced concrete structures

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Key Words: Damping, Reinforced Concrete, Dynamic, Nonlinear Model, Energy Balances

Earthquake events in recent years and their consideration in performance-based design have lead to the development of increasingly sophisticated physical models in structural computations. The nonlinear seismic behaviour of reinforced concrete (RC) structures is classically modeled through dissipative phenomena at two scales. At the material scale, nonlinear models describe some phenomena, such as concrete damage, friction, unilateral effects or plasticity. At the global scale, for dynamic analyses, energy dissipation is practically modelled with equivalent viscous damping.

To improve the description of energy dissipations when a nonlinear behaviour is considered, updated damping models are developed in literature usually based on the tangent stiffness matrix [2]. In this paper, a locally updated damping model is proposed based on the evolution of nonlinear variables such as concrete damage or friction. The model is first studied with a single degree-of-freedom (SDOF) model of a RC beam ($6\,\mathrm{m} \times 0.4\,\mathrm{m} \times 0.2\,\mathrm{m}$) showing accurate performances. Then, the construction of the matrix for a multi-fibre RC beam model is developed. Numerical analyses are then carried out to compare the performances of the proposed damping model with respect to more classical ones, as for example the Rayleigh damping model updated with the tangent stiffness matrix. The reference results are based on the experimental campaign carried out by T. Heitz [1]. A peculiar attention is given to the degradation of the beam according to frequency drop off. The evolution of the energy dissipations according to the degradation is investigated.

Finally, the proposed model is an improvement to classical damping models, such as Rayleigh ones, in terms of dynamic responses by dissipating more energy at the material level. The locally updated damping model is particularly improved by an explicit consideration of friction across cracked components.

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Numerical Evaluation of Bell-Shaped Proportional Damping Model for Softening Structures

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Key Words: *Proportional Damping, Bell-Shaped Model, Softening Response, Negative Stiffness*

In the modelling of large-scale structures, energy dissipations not already accounted for using material hysteretic models, often called un-modelled damping, are usually incorporated using viscous damping such as Rayleigh damping due to mathematical convenience and computational efficiency. The use of the Rayleigh damping model during inelastic response after yielding occurs could, however, lead to large spurious damping forces in the order comparable to material constitutive forces. This problem has been well-documented and studied [e.g. 1, 2, 3].

Many remedies have been proposed to address the spurious damping forces. However, most of them are not computationally efficient, and some also deviate from the idea of modal damping ratio due to loss of proportionality, resulting in difficulty for model parameter calibration against experimentally measured modal damping ratios. Most models are also not suitable for structures experiencing softening response due to having negative damping ratio.

A new type of proportional damping models, called bell-shaped proportional damping model, has recently been proposed [4]. This new model has not only addressed the spurious damping forces, but also maintained the same order of computational efficiency as the Rayleigh model. This model has also been further improved such that, by using the tangent stiffness approach, it becomes suitable for structures experiencing softening response with negative stiffness [5]. The improved model, called Type 4, allows users to have flexible control of modal damping ratio for all interested frequency intervals, including those associated with negative stiffness.

In this study, the performance of the Type 4 damping model is evaluated numerically in a response history analysis of a multi-storey building under seismic loading. The results show that, compared to the Rayleigh model, the Type 4 model performs excellently in terms of always giving desirable positive energy dissipation even when the structure is experiencing softening response.

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Classification of Seismic Failure Modes of Deep Steel Columns Using Machine Learning

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Key Words: *Machine Learning, Artificial Intelligence, Steel Deep W-shape Columns, Failure Mode Classification*

Machine learning approaches have received significant attention over the past few years in the field of civil engineering in general, and earthquake engineering in particular. Examples of their use in earthquake engineering can be found in Sediek et al. [1]. Generally, machine learning (ML) is a subset of artificial intelligence (AI) that uses sample datasets (i.e., training data) to tune the parameters of mathematical models which can be used to predict the response of new datasets that were not explicitly programmed in the mathematical models. Predicting the seismic failure mode of deep steel W-shape (DSW) columns is a potential application for such approaches in earthquake engineering. DSW columns can either fail in a global mode when subjected to an earthquake, where the column collapses globally with no plastic hinges at its ends; in a local mode, where the column fails due to the formation of "local" plastic hinges at its ends; or in a couple mode involving both local and global failure modes. Predicting the seismic failure mode of DSW columns is a challenging task due to its highly nonlinear decision surfaces that depend on many continuous and categorical parameters including geometric properties, boundary conditions and loading. Nevertheless, it is important for designing new DSW columns or deciding retrofit and rehabilitation strategies for existing DSW columns to predict their seismic failure modes. Therefore, this study explores the use of machine learning (ML) to predict the seismic failure mode of DSW columns. Steel Column Net (SCNet), a dataset of more than nine hundred experimental and numerical results of deep wide flange (W-shape) columns with different attributes is compiled. Three failure modes are distinguished in SCNet: local, global, and coupled modes. The efficiency of five machine learning (ML) classification models is explored to identify the failure modes of columns subjected to combined axial and lateral loading in a randomly assigned test set from SCNet. Among the ML classification techniques used, support vector machine and decision trees provide the best performance with a prediction accuracy of 89%.

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Collapse Assessment of Steel Buildings with Deep Columns under Tri-directional Seismic Excitations

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Key Words: *Collapse Fragility, Risk Assessment, Deep Columns, Steel Buildings*

Deep, wide-flange columns have been widely used in steel building in the U.S. because of the high stiffness and strength-weight ratio. While the structural instability of deep columns has been extensively studied at the member level, the influence of out-of-plane displacement and vertical ground motion on collapse behaviour of space frames with deep columns is not yet explored. To address this shortcoming, the collapse risk assessment of four-story steel planar and space frames under various seismic excitations is computationally investigated. High-fidelity finite element models are employed and analysed using explicit dynamic solver to capture instability and collapse behavior in the frames. Simulation results suggest that adding another horizontal ground motion is severely detrimental to the collapse capacity of space frames under all ground motion sets, while the effect of vertical ground motion is significant only when it changes the collapse mode. Moreover, composite slab combined with gravity frames can greatly reduce the collapse risk. However, gravity frames could induce vertical collapse due to buckling of gravity columns or facture in shear connections. Based on the results, the currently available design recommendations for the use of deep steel columns in steel buildings are evaluated and further revised.

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Effects of Longitudinal Reinforcement and Aspect Ratios on Deteriorated Hysteresis Behaviours of Reinforced Concrete Bridge Columns

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Key Words: *Reinforced Concrete, Bridge Column, Longitudinal Reinforcement, Aspect Ratio, Hysteresis Behaviour, Deteriorations, Hysteresis Model*

To study the effects of longitudinal reinforcement and aspect ratios on the deteriorated hysteresis behaviours of reinforced concrete (RC) bridge columns, five rectangular RC column specimens with hoop and tie reinforcements are tested under cyclic loading considering longitudinal reinforcement ratios of 0.75%, 1.5%, and 3.0% and aspect ratios of 3, 6, and 10 [1]. Furthermore, another five circular RC columns with spiral reinforcement and similar test scheme obtained by Leman and Moehle [2] are included to further compare the differences of deterioration characteristics resulting from various confining mechanisms. The deterioration characteristics are quantified and extracted from the test results through the calibration of a smooth hysteresis model [3] where each model parameter can represent a specific structural property. Test results show that the stiffness degradation and pinching severity of column would increase as its longitudinal reinforcement decreases. The pinching severity of column would also increase with decreasing aspect ratio, but the stiffness degradation is barely affected by the aspect ratio. Moreover, due to the well confinement effects, the severity of deteriorations of circular columns are less than those of rectangular columns with the same longitudinal reinforcement ratio and the minimum transverse reinforcements required by seismic design codes. Besides, the failure of rectangular columns is mainly caused by the loosening of transverse reinforcements at seismic hooks, leading to gradually deteriorated confinement and strength. In contrast, the failure of circular columns is primarily induced by the fracture of spirals, resulting in destruction of confinement mechanism and sudden strength loss.

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Influence of Position of Decks on Seismic Behaviour of Scissors-type Bridge

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Key Words: *Emergency Bridge, Scissors-type Bridge, Seismic Behaviour, Reinforcement Effect*

The Scissors Bridge is a deployable bridge designed for early bridging after a disaster [1]. By using a scissors structure for its main frame, the bridge can be transported in the assemble state, and it enables to reduce the number of workers and heavy machinery. Previous design studies have shown that the main frame of the scissors bridge is strongly affected by the bending moment [2]. It was also found that the effect of this bending moment could be reduced by installing the decks on the shafts in each scissor unit [3]. However, the reinforcing effect of the decks according to their position has not been fully clarified. In addition, it is necessary to clear the seismic performance of the scissors bridge considering used at disaster sites.

In this study, a parametric FE analysis was conducted in order to investigate the seismic performance of the scissors bridge focusing on the boundary conditions and the number of scissors units. Two different types of seismic waves, *the Kobe Earthquake* and *the Tohoku Earthquake*, were used for the scissors bridge with difference decks position: one is the deck type of bridge which was installed the decks on the upper shafts, and the other is the through type of bridge which was installed the decks on the bottom shafts.

The dynamic response factor of displacement and cross-sectional force was evaluated by comparing the results between static analysis and seismic response analysis. In case of the deck type of bridge, the dynamic response factor of the axial force increased from 10% to 30%. On the other hand, the dynamic response factor of the bending moment decreased from 20% to 40% compared to the case without decks. In case of the through type of bridge, the dynamic response factor of axial force decreased from 30% to 60%, but the dynamic response factor of the bending moment increased from 10% to 20% compared to the case without decks. From these results, it was found that so effective installing position for the axial force was the through type of bridge and for the bending moment was the deck type of bridge from the point of reducing the effect of its sectional force during the earthquake.

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15th World Congress on Computational Mechanics (WCCM-XV)
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A METHODOLOGY FOR INCLUDING SUSPENSION DYNAMICS IN A SIMPLE CONTEXT OF RAIL VEHICLE SIMULATIONS

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Key Words: secondary suspensions, dynamic stiffness, flexible carbody, rail vehicle dynamics.

Abstract. *The running behaviour of rail vehicles is highly influenced by suspension components. Dealing with ride comfort, secondary suspensions are adopted to reduce the vibrations transmitted to the carbody. In this context, the dynamics of the suspension elements themselves has to be properly included in multibody system. This paper proposes a strategy for modelling the passive vertical secondary suspension in the frequency domain. To this aim, a mathematical model is defined and its parameters are tuned to be representative of a real system. Then, a sensitivity analysis over the model parameters is proposed to discuss the suspension performances in terms of dynamic stiffness. Finally, a finite element model of the carbody is considered and coupled to the rear and front suspensions. The model is adopted to simulate the vehicle running on a rail track irregularity in the frequency domain, in the 0-30 Hz frequency range.*

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A semi-analytical method for random vibration of bogie-track-tunnel-soil interaction system

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Key Words: Frequency Response, Railhead Roughness, Uncertainty, FEM, Fourier Series

In order to understand the dynamic behavior of subway track and tunnel, it is important to evaluate the coupling system composed of train, track, tunnel and soil adequately. Railway vibration originates from the geometric and parametric excitations. The former, which may dominate the vibration, is induced by irregularities on the railhead and wheel tread. Since, in general, these profiles have uncertainties, the dynamic behavior is characterized by a random vibration. Therefore, the dynamic response should be assessed based on its average. In the case of conventional numerical methods, the dynamic interaction analysis is carried out for a given roughness generated over a finite range of the track model. Although the expected value of frequency spectrum can be approximately evaluated by smoothing over each 1/3 octave frequency band, this operation leads to a reduction in frequency resolution.

This paper presents a semi-analytical method for bogie-track-tunnel-soil dynamic interaction problems. The tunnel is modeled as an infinite cylindrical shell surrounded by an elastic region. The track is given by a periodically supported infinite rail. The railhead roughness is considered as a random process. Due to the periodicity of the track, the Floquet transform is applied to the interaction problem. Moreover, in order to reduce computational effort, the solution is represented by a Fourier series in the track direction [1]. Sections of the concrete slab and tunnel invert are discretized by finite elements. To evaluate the mathematical expectation of dynamic response, the relation between the power spectrum density of the roughness and the expected value of energy spectrum density (ESD) of acceleration at observation points inside the tunnel is derived explicitly [2]. It is found that the expectation of ESD is characterized by the superposition of vibrations originating from two wheelsets of a bogie.

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Assessment of the pantograph-catenary current collection quality by using indirect measurements and Artificial Neural Networks

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Key Words: *ANN, Artificial Intelligence, Catenary, Interaction Force Measurement, Pantograph*

Current collection in high-speed trains is usually carried out by means of the sliding contact between the pantograph collectors and the catenary contact wire. This pantograph-catenary interaction force directly determines the current collection quality, which is usually characterised by some statistical parameters. High contact forces tend to accelerate wear on both contact wire and pantograph collectors, while low contact force values may eventually produce arcing with its consequent negative effects. For that reason, European standards [1] limit certain parameters such as the mean, minimum and standard deviation of the interaction force.

The current collection quality of a given pantograph-catenary couple is commonly assessed by direct measurements of the interaction force. This implies to use an instrumented pantograph and perform specific in-line tests which are generally costly. To alleviate the drawbacks that this procedure entails, in this work we propose a methodology to predict the main statistical indicators that quantify the current collection quality based on indirect measurements and artificial intelligence techniques. Specifically, Artificial Neural Networks (ANN) are trained from the vertical acceleration of the pantograph collector head, which is relatively easier to measure in practise.

In this work, the pantograph accelerations have been numerically obtained from thousands of simulations of the pantograph-catenary dynamic interaction problem with the efficient algorithm proposed in [2]. These simulations are performed with different pantograph velocities and different contact wire height profiles to account for installation errors present at actual catenaries. The good prediction accuracy of the trained ANN shows that the proposed methodology can be an appealing alternative to the in-line contact force measurement for current collection assessment.

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Iterative algorithm to perform HIL tests with a periodic finite element catenary model

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Key Words: *Hardware in the Loop, Pantograph, Catenary, Periodic Models, Steady State*

Hardware-In-the Loop (HIL) testing has emerged as an appealing procedure to simulate the dynamic interaction between a real pantograph and a virtual catenary. In these tests, the pantograph contact strips interact with a linear actuator that simulates the catenary contact point. The interaction force is measured by load cells for feeding a numerical model of the catenary which provides the contact wire height profile that must reproduce the linear actuator. The aim of these tests is to replace homologation in-line tests, thus reducing the homologation cost.

To carry out HIL pantograph tests it is mandatory to solve the dynamic behaviour of the catenary model in real-time. This requirement usually leads to simplified models to describe the catenary system that limit the accuracy of the results [1]. In this work, we propose a complete framework to perform HIL pantograph tests by using a periodic catenary finite element model. This model only accounts for the steady-state regime, which is very representative of the general behaviour of the high-velocity pantograph-catenary interaction. In those catenaries, long straight sections with very similar spans are commonly installed. To achieve the steady-state solution in the HIL test rig, an iterative strategy is also described and numerically validated [2].

One of the main advantages of the model proposed is its ability to consider the non-linear behaviour of droppers, which slackens under compressive forces. Furthermore, actuator control-loop and sensor delays can be easily handled. The results obtained from HIL tests are compared to those obtained from pure simulations showing good agreement. Finally, an optimized catenary geometry has been tested in the HIL test rig to validate if the optimized model still behaves in an optimal manner when interacting with a real pantograph.

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Modelling of Innovative Yaw Dampers for Railway Vehicles

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Key Words: *Railway Dynamics, Yaw Dampers, Multibody Dynamics, Vehicle Stability, Curve Negotiation*

Nowadays, the tendency to increase the competitiveness of railway vehicles by raising their commercial speed is widely diffused around the world. Such enhanced velocity levels must be reached without decreasing the standard safety levels.

Considering the straight track condition, yaw dampers are the most influencing secondary suspension components of the railway vehicle able to increase the stability during high-speed operations [1], [2]. The dampers contribute reduces the risk of hunting instability and, therefore, it increases the vehicle critical speed. The typical passive yaw dampers are designed to achieve this goal, but, unfortunately, they worsen the curving performances [3]. Indeed, the forces provided by the standard passive devices increase the bogies steering resistance during the negotiation of sharp curves, especially along curve entries and exits, with a consequent increase of the wheel-rail contact forces.

For this reasons, damper manufacturers are studying innovative solutions to modify the internal characteristics of the dampers according to the vehicle working conditions. The goal is to obtain devices able to combine the vehicle stability during the high-speed running and the curving performances in sharp curve negotiation.

In this context, the present work aims at developing a numerical model of the new yaw dampers, validated with experimental results collected on a specific test bench. Then, the numerical evaluation of the vehicle performances with the innovative yaw dampers is carried out by a co-simulation routine: a multibody vehicle model of a real test case, implemented in the Simpack® software, is run together with a Simulink® model of the yaw damper. The performances are analysed taking inspiration from the EN 14363 standard in terms of both high-speed running stability and low speed curve negotiation.

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Uncertainty Quantification for High-speed Train Dynamics Modeling and Optimization under Uncertainties to Limit Energy Consumption

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Key Words: Optimization under uncertainties, Bayesian inference, High-speed train dynamics

Controlling the energy consumption is an important stake in today's world. In the railway field, the energy consumed by high-speed trains depends on many variables such as the driver behaviour. Significant variations have been noticed for different drivers on the same journey. To help drivers, crossing points are defined along the journey, but differences still exist. The industrial objective of this work is to define a model, able to describe the train dynamics and to propose an optimization method, which aims to minimize the energy consumption.

This work is composed of two parts. First, a deterministic model is defined to describe the train longitudinal dynamics based on a Lagrangian approach [1]. This model is calibrated based on commercial trains measurements. Afterwards, the optimization of the command is performed using the CMA-ES method [2] to minimize the energy consumed while punctuality, security, and comfort constraints are respected. Nevertheless, the high-speed train system is complex, and taking into account the uncertainties of the model parameters is necessary. Therefore, a Bayesian inference method [3] is applied in order to include uncertainties in the previous deterministic model. Finally, an optimization under uncertainty method is used to find the optimal command.

The originality of this work lies on its transposability to real train systems. Indeed, pneumatic braking is distinguished from dynamic braking (able to recover a part of the energy consumed). The optimization method is applied to the driver command and it combines both punctuality and physical constraints. Many energy measurements are used to calibrate and validate the models and verify the quality of the optimal solution. Finally, the rolling environment of the train is determined carefully by the use of wind predictions, track declivity and curvature measurements.

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Multi-element polynomial chaos with automatic discontinuity detection for nonlinear systems

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Key Words: Polynomial Chaos, Multi-element, Discontinuity Detection, Polynomial Annihilation, Support Vector Machines, Uncertainty quantification.

Generalized Polynomial Chaos expansion (gPC) is a well-known method for uncertainty quantification of stochastic systems, in particular for smooth responses [1]. In the case of nonlinear systems exhibiting discontinuities in their surface response, it has been demonstrated that multi-element generalized polynomial chaos (ME-gPC)—which is based on an element decomposition of random space—provides accurate results. However, the definition of the elements, a key step of ME-gPC, is usually based on a tensor structure and the number of elements increases dramatically at high stochastic dimension [2]. In this study, the focus is made on the decomposition of the random space for nonlinear mechanical systems in order to efficiently apply gPC with a limited number of elements. More specifically, this decomposition relies on an automated detection procedure of the surface response discontinuities (referred to as *edges*) represented by cubic-spline curves. The proposed edge tracking detection is first detailed and validated on analytical test cases. Then, a specific implementation of ME-gPC is presented so that it may be efficiently applied on elements whose frontiers are defined by four cubic-splines in order to maximize the versatility of the random space decomposition. Finally, the proposed methodology is applied to the analysis of an academic Duffing system and an industrial compressor blade, NASA rotor 37, featuring blade-tip/casing contacts [3]. It is shown that the proposed developments yield accurate results both for the discontinuity detection and the response approximation in comparison to the reference Monte-Carlo simulations.

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Nonlinear geometrical dynamics of cyclic symmetry structures: application to bladed disks

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Key Words: *Internal resonance, Harmonic Balance Method, geometric nonlinearities, reduction model, cyclic structure*

The development of new aircraft engine architectures is mainly focused on performance and energy efficiency. One way to achieve this objective is to reduce its weight by using composite materials but also to increase the by-pass ratio of these machines. These last two points lead to long and thin, and therefore very slender blades geometry. Such designs make these structures more flexible, which can then exhibit non-linear geometric behaviours. This geometry combined with the cyclic symmetry property of the bladed disk will generate specific non-linear behaviours such as non-linear energy localization or even internal resonances. Using a non-linear curved beam model taking into account large displacements, twist change and a profiled cross-section [1], we have been able to study the non-linear contributions of each term of the model and thus to have a good understanding of the involved physics. All of these simulations were carried out taking into account the effects of rotation on the beam. Finally, a numerical approach has been developed to deal with large models such as those encountered in industry. The strategy developed is based on non-linear reduction approaches adapted to geometric nonlinearities such as modal derivatives [2], companion modes [3] or normal form [4] of the motion equations. These results were compared to experimental data that allowed to validate the developed approaches. It should be noted that this work also made it possible to take advantage of the non-linear behaviour of the structure by using the properties of internal resonances. Indeed, we were able to decrease the level of vibration by transferring energy from one mode to another with better dynamic characteristics.

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Probabilistic Learning Based Optimization of the Detuning of Bladed-Disks in Nonlinear Stochastic Dynamics in Presence of Mistuning.

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Key Words: Bladed-disk, Detuning, Mistuning, Finite displacements, Uncertainty Quantification, Combinatorial optimization, Probabilistic learning on manifolds

The vibrational behavior of bladed-disks is known to be particularly complex in reason of mistuning amplifications but also in reason of geometrical nonlinear effects (use of lighter materials). In such a context, methodologies for the dynamical analysis based on the nonparametric probabilistic approach [1] odf the random mistuning combined to nonlinear reduced-order models allows for a better understanding of uncertainty propagation through the forced response [2]. The difficulty related to this unavoidable mistuning effects has led to consider the detuning (alternating between several blade types) as a way for inhibiting the amplifications. A computational methodology adapted to the detuning context of nonlinear dynamics of mistuned bladed-disks developed in [3] has shown very encouraging results. In this context, the present research deals with a novel formulation for the detuning optimization of a bladed-disk structure using a 12 bladed-disk computational model issued from [4]. The dynamical amplification is defined with respect to the pure mistuned configuration and involves scalar quantities that are defined from the extreme values of the maximum displacements occurring in the structure. The numerical procedure allows for obtaining a full data basis. Its analysis shows the existence of a few number of detuned configurations that reduce the mistuning amplification effects. A second part of this work consists in proposing a formulation of the combinatorial optimization problem for which a surrogate model of the cost function is constructed using the PLoM method [5], as a machine learning tool from a small training set. The optimal solution obtained is compared to the one obtained with the data basis.

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Reduced Order Modeling of Cyclically Symmetric Bladed Disks with Geometric and Contact Nonlinearities

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Key Words: Reduced Order Modeling, Geometric Nonlinearities, Rotor/Stator Interaction

In the current economic and environmental context, aircraft engines manufacturers try to design more efficient engines in order to reduce their fuel consumption. First, aerodynamic losses are decreased by reducing the clearance between the blades and the surrounding casing. This can lead to contact events between the blades and the casing even in nominal operating conditions [1]. Then, the engine weight is reduced by designing lighter, and therefore more flexible, blades. As a consequence, the blades can undergo large displacements and deformations [2].

A methodology has been recently derived to study the contact interactions of single blades undergoing large displacements [3]. In this article, this methodology is extended to full bladed disks with cyclic symmetry. In order to be computationally efficient and compatible with the use of large industrial models, the methodology is based on a reduction procedure. Each sector of the high fidelity model is projected onto a basis composed of Craig-Bampton modes and a selection of their modal derivatives. The internal nonlinear forces due to large displacements are evaluated in the reduced basis with the stiffness evaluation procedure [4]. Contact is numerically handled with Lagrange multipliers.

The numerical strategy is applied on an open industrial compressor model, the NASA rotor 37, in order to promote reproducibility of results. This work demonstrates that reduced order models provide a computationally efficient alternative to full order finite element models for the accurate prediction of the time response of structures with both distributed and localized nonlinearities.

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Dynamic Simulation of Vehicle-Bridge Interaction Using a Novel Simple Analysis Procedure with Composite Time Integration Method

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Key Words: *Implicit Dynamic, Composite Time Integration Scheme, Equivalent Node Secant, Frame Element, Vehicle-Bridge Interaction*

In order to simulate the vehicle-bridge interaction by using a numerical model with high stiffness elements for a long duration, Bathe composite time integration scheme is incorporated into the new implicit dynamic finite element analysis procedure proposed by Lee et al. [1-2] in this study. The Bathe scheme can be viewed as an extension of the trapezoidal rule in which the trapezoidal rule is combined with the 3-point Euler backward method. When analysing nonlinear dynamic problems with large deformations, long duration, and high stiffness elements, Bathe scheme demonstrates its simplicity and accuracy in previous studies [3-5]. On the other hand, the new analysis procedure introduced the concept of equivalent node secant coefficient to decouple the governing equilibrium equations so that the factorization of an effective matrix is no longer necessary. Compared to the traditional implicit dynamic finite element procedure, the new analysis procedure dramatically saves much computation time and possesses high reliability and accuracy as shown in the previous study. In particular, any kind of FE can be included in the analysis procedure as long as the element internal and damping nodal forces can be exactly evaluated.

High stiffness contact element can be used to simulate the vehicle-bridge interaction during nonlinear dynamic analysis. When a vehicle-bridge interaction system is subjected to extreme earthquake, highly nonlinear and discontinuous dynamic behaviour, such as vehicle uplift, collision and derailment, may occur. The hybrid integration method proposed in this study can effectively maintain the convergence and stability of the 3D numerical analysis. Finally, the vehicle-bridge interaction model is constructed by space truss/frame with high stiffness contact element. The analytical results obtained by proposed method are compared with those obtained by traditional implicit method to verify the accuracy and efficiency of the proposed hybrid integration method.

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Simulation of High-Speed Railway Bridges under Strong Earthquakes Using a New Dynamic Analysis Procedure

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Key Words: *Vehicle-Rail-Bridge Interaction, Wheel Rail Contact, Finite Element, Nonlinear Dynamic Analysis*

Railway technology has been developing rapidly and the number of long-span railway bridges has been increasing. A long-span and heavy railway bridge may result in obvious vehicle-rail-bridge interaction due to its flexibility property and heavy dead load, especially for high-speed railway bridges under strong earthquakes. The purpose of this study is to simulate the vehicle-rail-bridge interaction of high-speed railway bridges under strong ground motions by using a new implicit dynamic finite element analysis procedure proposed by Lee et al. [1-2].

It is very difficult for traditional finite element analysis procedure to deal with problems with large deformation, collision, fracture, high velocity, high non-linearity and discontinuity. The new implicit dynamic finite element analysis procedure does not require assembling the structure stiffness and damping matrices. Without the factorization of an effective matrix, the computation efficiency is greatly superior to that of conventional implicit methods. Any kind of FE can be included in the analysis procedure as long as the element internal and damping nodal forces can be exactly evaluated. Therefore, the new dynamic finite element analysis procedure is used to simulate highly nonlinear and discontinuous dynamic behavior of long-span bridges as well as high-speed moving vehicle loads under strong earthquakes.

When a high-speed railway bridge is subjected to extreme earthquake, highly nonlinear and discontinuous dynamic behavior, such as vehicle uplife, collision and derailment, may occur. In this study the 3D simulations of vehicle sub-structures, moving loading, wheel-rail contact, vehicle uplife are developed and included in the new dynamic analysis procedure. Through extensive simulations of single-span long-span bridges, the obtained results are compared with the current design formula. The bridge seismic design, train design load mode and reasonable speed limit for long-span bridges are discussed.

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Simulation of Vehicle-Bridge Interaction Using a Novel Dynamic Analysis Procedure with Geometrically Nonlinear Solid Elements

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Key Words: *Implicit Dynamic analysis, Eight-Node Hexahedral Element, Rigid Body Motion, Vehicle-Bridge Interaction, Bridge Deck*

This study is aimed at the simulation of vehicle-bridge interaction using a novel dynamic analysis procedure with geometrically nonlinear solid elements. The bridge deck is idealized by solid elements to investigate the concentrated stress in the deck while a heavy vehicle is passing through the bridge. Compared with the traditional implicit dynamic finite element procedure, the new implicit dynamic finite element analysis procedure proposed by Lee et al. [1-2] does not require assembling the structure stiffness and damping matrices. Without the factorization of an effective matrix, the computation efficiency is greatly superior to that of conventional implicit methods. Any kind of FE can be included in the analysis procedure as long as the element internal and damping nodal forces can be exactly evaluated. Therefore, the novel dynamic analysis procedure is adopted in this study.

A geometrically nonlinear eight-node hexahedral solid element is developed and included in the novel dynamic analysis procedure. The rigid body motion of the eight-node hexahedral element is subtracted from the total displacement based on co-rotational coordinate systems. After the pure deformation is determined, engineering strain and engineering stress can be applied to calculate the internal nodal forces. The proposed approach is more efficient than that using the Green-Lagrange strain and the second Piola-Kirchoff stress in geometric nonlinearity problems. Compared with the traditional finite element method for nonlinear geometrical structures, the proposed method can significantly reduce computation time. In addition, according to the previous researches this dynamic analysis procedure demonstrates high reliability and accuracy in large deformation structures. The analytical results obtained by using the developed element are compared with those obtained by ABAQUS software to verify the accuracy and efficiency of the proposed solid element. Finally, the stress distribution of the bridge deck while heavy vehicle passing through is investigated.

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Spatial-varying frequencies for a beam subject to a moving vehicle

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Abstract

Compared to conventional bridge structure with pier supports, the steel box-girders suspended by bracket structures of a monorail is flexible for most monorail transit system. Thus, as a train carriage travels on a series of flexible hanged box-girders, the vibration of train-monorail system can be regarded as the topic of *a heavy vehicle traveling on a light beam*. Obviously, the inertia effects of moving masses on dynamic response of a monorail would become significant. In this study, the spatial-varying of nature frequencies of a beam subjected to a moving mass will be conducted. On the other hand, as a high speed train moving on a bridge with resonant speeds, such a dynamic phenomenon would become noticeable once the VBI effect is taken into account for performing the interaction dynamic analysis of a train-bridge system. The numerical results revealed that the resonant speed would be slightly shifted to lower speeds due to the inertia effects of the train cars traveling on the bridge.

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A Design Digital Twin For Metallurgical Process Development In Directed Energy Deposition Additive Manufacturing

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Key Words: *Digital Twins, Directed Energy Deposition, Additive Manufacturing, Multiscale modeling*

Digital process development for additive manufacturing is emerging as a sustainable, cost-attractive alternative to the traditional experimental trial-and-error approach whereby computer modeling and simulations are used to explore the process window for a given material, 3D printer, and part. At the same time, digitalization is a hard task requiring validated, high-fidelity models at different length scales (part and melt pool) and time scales (solidification to build time). Such challenges are equally valid for directed energy deposition (DED), which is typically characterized by a laser head following the movement of a robot code (g-code) to build the component. Here, we report on our efforts to achieve a design digital twin for the DED process by developing a fully in-house integrated model including thermal simulation at the scale of the part, classification of thermal history to identify key locations in the component, microstructure evolution, multi-bead multi-layer deposition of material, phase fraction model at the scale of the part including nonlocal mechanical properties, and residual stress and distortion. By using such design twin, users are able to explore the role of process parameters as well as of gcode, therefore developing the process to optimize the final part's microstructure, mechanical properties, and distortion.

A mixed interface-capturing and interface-tracking CFD framework for modeling metal AM processes at different scales

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In this talk, we present a novel computational framework by mixing interface-capturing/interface-tracking methods for simulating the thermal multi-phase flows in metal AM applications, focusing on better handling the gas-metal interface, where AM physics, such as phase transitions and laser-material interaction, mainly takes place. The framework, built on level set method and variational multi-scale formulation (VMS), features three major contributions: (1) a simple computational geometry-based re-initialization approach, which maintains excellent signed distance property on unstructured meshes, re-constructs an explicit representation of gas-metal interface from the level set, and facilitates the treatment of the multiple laser reflections during keyhole evolution in AM processes; (2) a fully coupled VMS formulation for thermal multi-phase governing equations, including Navier-Stokes, level set convection, and thermodynamics with melting, solidification, evaporation, and interfacial force models; and (3) a three-level recursive preconditioning technique to enhance the robustness of linear solvers. We first compare the geometry-based re-initialization with the Eikonal partial differential equation (PDE)-based approach on two benchmark problems on level set convection and bubble dynamics. The comparison shows the geometry-based approach attains equivalent and even better performance on key criteria than the PDE-based counterpart. We then apply the developed framework to simulate two AM experiments, which Argonne National Laboratory has recently conducted using in-situ high-speed, high-energy x-ray imaging. The proposed framework's accuracy is assessed by thoroughly comparing the simulated results against experimental measurements on various quantities. We also report important quantities that experiments can not measure to show the modeling capability.

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A semi-analytical thermal modelling approach for multilaser powder bed fusion

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Key Words: Multi-laser, Cost efficient thermal modelling, Scanning strategy, Semi-analytical model.

The low production speed and limited part size are two critical limitations in laser powder bed fusion (LPBF) of metallic components. On the other hand, multilaser powder bed fusion e.g.[1] has been effective in improving productivity and reducing production time, thus allowing for the manufacturing of larger components. It is well known that the multi-laser powder bed fusion process parameters and the laser scanning strategy have a substantial effect on the temperature transients of the part and henceforth on the degree of deformations and residual stresses. LBPF process models can be instrumental in determining the optimal process parameters.

Ideally, the process model needs to be both accurate and computationally tractable. However, the LBPF process is a complicated multi-physics problem to analyse, which also requires a due account for the geometry of the part to be built. Since the thermal expansion/contraction cycles are critical for the part distortion and residual stress field, it is crucial to determine the temperature transients accurately. The steep temperature gradients are present due to the local nature of heating. The laser beams have a spot radius typically of tens of micrometres, while the parts produced have dimensions typically of tens of millimetres. This mismatch of characteristic length scales becomes prohibitive when a numerical scheme such as finite elements is used to solve the governing heat equation. This would require fine spatial and temporal discretisation to resolve the steep temperature gradients, which in turn requires an excessive number of elements and time steps, resulting in very high computational costs.

A semi-analytical thermal model [2] of the multi-laser powder bed fusion process is presented, which determines the temperature evolution by representing the moving laser spot with a finite number of point heat sources. The solution of the thermal problem is constructed from the superposition of analytical solutions for point sources and complementary numerical/analytical fields to impose the boundary conditions. The unique property of the formulation is that the numerical discretisation of the problem domain is decoupled from the steep gradients in the temperature field associated with localised laser heat input.

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Additive Manufacturing: From Nonequilibrium Interfaces to Strange Grains

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Key Words: Rapid solidification; additive manufacturing

A major challenge with classical rapid solidification processing, such as melt spinning or pulse laser melting, is the difficulty in producing three-dimensional parts that retain the novel microstructures produced by rapid solidification. However, with the advent of additive manufacturing (AM) it is possible to create objects with rapidly solidified microstructures. The interfacial velocities and temperature gradients found during AM are much different than in traditional castings, with high solidification rates (10^{-3} - 1 m/s) and high thermal gradients (10^5-10^7 K/m). These solidification and cooling rates can lead to ultra-fine microstructures and unexpected metastable phase formation. The presence of large thermal stresses can lead to hot-cracking and plastic deformation of the as-solidified metal alloy. Moreover, the highly directional nature of the solidification process yields very unusual grain structures. All these issues can have a major effect on the resulting properties of the part. Following an introduction of the challenges of predicting AM microstructures, a discussion of the development of grain structure during powder bed AM of stainless steel 316L will be given. The large-scale phase field simulations of the morphological development of grains illustrate the complicated interaction between interfacial mobility anisotropy, weld pool shape, laser scan strategy and multiple powder layers on the resulting grain morphology. A phase field model that is designed for the interfacial velocities characteristic of AM and allows the nonequilibrium properties of interfaces to be tuned for a chosen alloy system will also be discussed.

An Extended Cellular Automaton Finite Volume Method for Process-Microstructure Simulation of Wire-based Additive Manufacturing

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Key Words: *Additive Manufacturing, Thermal Fluid Flow, Grain Structure, Numerical Modelling*

Metallic additive manufacturing (AM) possesses tremendous advantages in building geometrically complex parts with tailorable microstructures and properties and thus has found potential to revolutionize the global part manufacturing landscape. Among many metallic AM technologies, wire-based AM is breaking size and weight barriers for heavy industries. However, due to many AM process parameters, trial-and-error experimentation for analysis and optimization is time-consuming and costly. Therefore, it is critical to developing individualized numerical methods for further understanding AM's process-structure relationship to guide and expedite the parameter optimization. This work proposes an extended cellular automaton finite volume method to simulate the wire-based melt pool, solidification, and grain evolutions during the wire-based AM. In the proposed method, we adopt the finite volume method for the thermal-fluid flow simulation, the cellular automaton for the grain nucleation and growth within the mushy zone, and the Motte Carlo Potts model for the grain coarsening in the heat-affected zone. The advantage of the proposed method over other integrated methods is that it resolves the grain coarsening in the heat-affected zone and considers the crystallographic orientation of the unmelted grains or nucleated grains in the Motte Carlo Potts model. We conducted a set of numerical examples of Ti6Al4V wire to demonstrate the proposed method's accuracy and capability and provide insights into the melting and solidification processes. A good agreement with experimental data in the literature shows that the proposed method is a valuable tool to simulate and analyze the process-microstructure relationship of the wire-based additive manufacturing process.

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Crystal Introducing Mechanism in Laser Wire Directed Energy Deposition Fabricated Ti6Al4V

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Key Words: *Solidification Microstructure, Metal Additive Manufacturing, Recrystallization*

ABSTRACT

Metal additive manufacturing (MAM) have been rapidly developed for almost twenty years, however, the mechanism of nucleation (or crystal introducing) mechanism in MAM processes has been a long-term unsolved problem. Only limited works shed lights on this area from experimental and simulation point of view, and no universal solution has yet been addressed. This work discusses the importance of nucleation in MAM and investigates the crystal introducing mechanism in laser wire DED fabricated Ti6Al4V. Besides the term 'nucleation', this phenomenon is generalized as the 'crystal introducing' because the crystals with different crystal orientations can be introduced to the printed domain without going through a nucleation scenario (growth from a successful critical nucleus in liquid phase). To investigate the crystal introducing mechanism in laser wire DED fabricated Ti6Al4V, a sample matrix under different fabrication conditions is fabricated under three hypothesises (stress, heat accumulation and the solid-state transformation). It is approved from different perspectives that the recrystallization is the main reason for the crystal introducing, and it is a comprehensive result of the residual stress and reheating. A more detailed investigation was carried out at the early stage of a recrystalized grain at the grain boundary of the prior beta grain boundary. The formation tendency of the recrystalized grain indicates its strong dependency on the grain boundary alpha phase. This study also approved that this type of recrystallization does not necessarily take place at the prior beta grain boundary area, even without grain boundaries, a single beta crystal can still be recrystalized into smaller grains under the fabrication condition of laser wire DED. Some of these recrystalized grains are able to participate into the following competitive grain growth, thus influence the solidification microstructure in the fabricated part dramatically.

Data-driven analysis of microstructure-property linkages for additively manufactured materials

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Key Words: *Microstructure Characterisation and Reconstruction, AM, Ti-Al6-V4, Fatigue*

Additive manufacturing (AM) has huge potential to manufacture optimal structures but is still in the state of ongoing research and development as small variations in the process can have a major impact on the resultant material in terms of volume defects, surface characteristics or microstructure. These, in turn, influence the mechanical properties. In order to exploit the full potential of AM, understanding the underlying process-structure-property linkages is crucial.
In this contribution, we propose a general framework to computationally investigate the microstructure-property relationships. As experiments alone are prohibitively expensive, computational augmentation is employed. This allows to create the large data bases for the adopted data-driven approaches which enable profound correlations. The proposed general framework consists of four steps:

1. two-dimensional microstructure images (from experiment or synthetic) are characterised by translation-invariant descriptors;
2. three-dimensional microstructures are reconstructed from the descriptors [1];
3. numerical simulations are conducted to compute mechanical properties [2];
4. descriptors and properties are correlated. Descriptors of further microstructures are identified for improving the quality of the correlation or for finding optimal properties. Back to step 2.

This framework is applied and presented for two examples: The optimisation with regard to fatigue performance of microstructures with variable position and morphology of hard precipitates and a fixed crystal microstructure as well as the prediction of fatigue performance of Ti-6Al-4V specimens based on CT scans of their pore microstructure. The results show the framework's capability of identifying an optimal structure for desired properties as well as the capability of predicting the properties for a given, unseen structure.

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Design and Printability Evaluation of Heat Exchangers with Respect to Laser Powder Bed Fusion Additive Manufacturing

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Key Words: *Heat Exchanger, Isogeometric Analysis, Topology Optimization, Residual Deformation Simulation, Laser Powder Bed Fusion*

Heat exchangers (HXs) have been widely used in various equipment and machines. It is very significant to implement structural design to improve heat exchange performance (HXP) and save energy accordingly. Topology optimization has been a popular methodology for this goal [1]. Moreover, additive manufacturing (AM) has been applied to practical fabrication of the complex HXs. In this work, the structural design and AM of cross-flow HXs are studied. A unit-based optimization framework is proposed to design the channel configuration in order to maximize heat exchange performance and meanwhile control pressure drop between the fluid inlet and outlet. A gradient-based optimization methodology is used. During the channel configuration evolution, for an intermediate design, filtering technique is adopted specifically to avoid sharp features and improve AM printability. Moreover, printability evaluation is considered for the optimized structures with respect to metal laser powder bed fusion (LPBF) AM process. Residual deformation is considered as an index to evaluate the printability. The entire HX containing the optimized thin-walled channels is modelled, and its residual deformation is predicted through sequential layer-by-layer simulation [2]. If weak printability is detected, some re-design work is added to the unit-based design. Finally, a new design can be achieved as the compromising solution that leads to better HXP (e.g., nearly 50% increase), limited pressure drop and good printability with respect to the LPBF AM process.

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Development of a Process Simulator thru GPU Acceleration and Adaptive Remeshing for Studying Porosity Variation in Laser Power Bed Fusion

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Key Words: *Additive Manufacturing, Process Simulation, Adaptive Remeshing, GPU*

As-built parts manufactured by laser powder bed fusion (L-PBF) suffer from the reduced fatigue strength due to the large pores caused by lack of fusion (lof) between scan lines. The lof porosity mainly depends on the melt pool size, which may change based on the geometrical features and scanning strategies, and process parameters. Unlike experimental approaches, process simulations (e.g. finite element analysis) can help deliver insights on the melt pool morphology, by which lof porosity can be estimated. Finite element method (FEM) based modeling approaches considering moving heat source can help predict the layer-by-layer lof porosity formation; however, they are computationally expensive as it requires large number of simulation steps, fine mesh to represent the powder layer and laser beam, and powerful computational resources.

This work presents the development of a computational framework to overcome the computational expense of simulating the L-PBF process. First, a matrix-free approach is used instead of the widely used global-matrix method utilizing high performance computing through (Graphical Processing Units) GPUs [1]. Second, an adaptive remeshing technique that significantly reduces the number of elements and nodes representing parts during the process is used. The power of using the matrix-free technique along with adaptive remeshing is demonstrated by performing detailed thermal process simulation for a relatively larger part using the moving heat source and true powder layer thickness where it was found that computational time could be reduced by at least 99%. In addition, two different parts and multiple scanning strategies are considered to show the influence of the scanning strategies and geometrical features (e.g. overhangs). The predictions are validated by experimental results.

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Development of Adaptive Smoothed Particle Hydrodynamics Method with Focus on Additive Manufacturing Simulation

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Key Words: *Additive Manufacturing; Multiphysics modeling; SPH; Adaptive; Refinement; Coarsening.*

Numerical simulation of Additive Manufacturing (AM) processes using the Smoothed particle Hydrodynamics (SPH) method is usually performed with uniform particle size. Despite many remarkable and promising results reported mainly in CFD applications (see in [1] and [2], for example), the use of spatially varying particle distributions in SPH AM simulation remains relatively unexplored. The authors of [3] laid the groundwork for modeling a multi-resolution AM simulation with SPH; nevertheless, their approach does not permit particle coarsening and is presented for 2D applications with only one level of refinement.

In this work, we develop a highly-efficient 3D SPH simulation framework for AM applications by enabling both particle refinement and coarsening procedures. To further enhance the computational performance of the method, an optimized neighbor-search algorithm for non-uniform particle size scenarios is also implemented into the in-house code. The robustness and efficiency of this approach are demonstrated by running the computer program on a single CPU core to simulate a multi-track Laser Powder Bed Fusion (LPBF) process. The present multiphysics modeling approach accounts for all relevant physical phenomena and melt-pool dynamics encountered in LPBF, such as material phase change, surface tension forces, recoil pressure, and Marangoni effects.

As a result of this SPH development, the fully adaptive 3D LPBF simulation can save more than 60% of the computational cost and is completed in a fraction of the runtime required for a similar single-resolution case. To achieve more efficient AM simulations using SPH, the development proposed in this work needs to be coupled with parallel computing algorithms so an additively manufactured part as simple as 1x1x1 mm can be modeled within a reasonable calculation time. Such an achievement would provide deeper insights into the underlying physics of the AM process of interest and allow for process monitoring and optimization.

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Extended One-dimensional Model for Efficient Mechanical Computation in Directed Energy Deposition Additive Manufacturing

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Key Words: Additive Manufacturing, Directed Energy Deposition, Residual stress, Extended One-dimensional Model

Residual stresses in directed energy deposition (DED) depend on the temperature history. Although fast numerical approaches have been developed for the thermal analysis [1], the efficient computation of residual stresses remains challenging, as 3D/2D finite elements (FE) method involves meshing along the layer thickness and/or height, which implies a very fine discretization along the print direction to avoid conditioning issues [2]. An alternative approach is proposed to significantly reduce computation time while capturing complex stress fields in the part. Since DED basically consists in adding a thin layer to the existing part, we propose an enriched 1D model immersed in the 3D space. Both layer thickness and height are internal parameters independent of the mesh size, which in turn can be coarser along the print direction. At each material point, 4 displacement vectors are introduced leading to 12 DOFs. Thus, kinematic conditions between a layer and its 4 neighbors (i.e., right, left, top and bottom) may be simply written. The model derivation through the virtual work principle will be broached, as well as a linear thermo-elastic behavior. In addition, several analytic calculations of multilayer structures representing both single and multi-track scanning strategies will be derived and used as exact references to validate a more general numerical implementation of the model. Future works will include the derivation of an elasto-plastic behavior and numerical optimization of the process parameters [3] based on the proposed 1D extended model.

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High-Fidelity Multi-Physics Modeling of Process-Structure-Property Relationships in Additive Manufacturing

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Key Words: *Additive Manufacturing, Multiphysics Modeling, Process-Structure-Property Relationships, High-Fidelity*

The wide adoption of additive manufacturing is hindered by the lack of comprehensive understanding of process-structure-property relationships. To this end, we have developed and seamlessly integrated a series of high-fidelity multi-physics models, including: physically-informed heat source models to shed light into manufacturing processes, microstructures, and mechanical properties [1]. Specifically, multiphase flow models using the coupled computational fluid dynamics (CFD) and discrete element method (DEM) simulate the powder spreading procedure and powder spattering and denudation phenomena in the powder melting procedure [2,3]. The powder melting model is powerful to reproduce the molten pool flow and relevant defects (e.g., lack-of-fusion and keyhole pores) by incorporating the major physical factors, especially the physically-informed heat source models, i.e., for an electron beam from micro-scale simulations of electron-atom interactions and for a laser incorporating multi-reflection and Fresnel absorption. The microstructure evolutions at both the grain- and dendrite- scales are modelled using the phase field [4] and cellular automaton methods [5]. The mechanical properties and thermal stresses are simulated using the crystal plasticity finite element (FE) model, which incorporates the realistic geometry (rough surfaces and voids), temperature profiles and microstructures [6]. These models have proven to be useful in revealing the physical mechanisms, which have been validated against experiments.

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Immersed Boundary Methods for Laser Powder Bed Fusion Process Simulations

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Key Words: *Laser powder bed fusion, Finite Cell Method, Two-level method, Multi-rate time integration*

The extreme scale ranges in both space and time involved in laser powder bed fusion (LPBF) process as well as the geometrical complexity of the parts produced by means of LPBF technology call for flexible numerical approaches. Therefore, immersed boundary methods seem to offer a valid alternative to the traditional mesh-conforming finite element method. In the present contribution, we adopt two methods of such a family of numerical methods to investigate some of the most challenging problems in LPBF simulations, namely the influence of process-induced defects and the spatio-temporal scale range.

A well established immersed methodology is the so-called Finite Cell Method (FCM), which has already been applied successfully in several contexts, from structural analysis to biomedical applications since it allows to easily deal with complex shape components otherwise non trivial or even impossible to mesh in a conform manner. In our contribution, we present the application of FCM in the context of high-fidelity thermal and thermomechanical analyses of LPBF processes. The proposed numerical scheme [1] is first validated with respect to experimental measurements of residual stresses taken from the literature and then applied to investigate the influence of lack-of-fusion defects on the melt pool morphology, providing a valuable tool to further understand the complex *process-structure-property* relationship in LPBF components.

Another promising immersed boundary technique is the two-level method, where the local and global scales of the problem are solved on two separate meshes weakly coupled in a way similar to a fat-boundary approach. To address the spatio-temporal scale range issues that burden LPBF processes simulations, we have combined the two-level formulation with a multi-rate time integration based on a predictor-corrector type scheme. Exploiting the peculiarity of the two-level method, we are able to treat differently - in a smooth and simple workflow - local and global effects in both the spatial and the temporal scale. We will present first the results of a thorough numerical verification of the proposed methodology on two- and three-dimensional problems, and then its application to a more challenging LPBF simulation, where we have observed a computational speed-up by a factor 4 compared to the spatial version of the two-level method with a monolithic time integration scheme.

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Modelling, and validation of Selective Laser sintering of PA12

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Key Words: *Selective Laser Sintering, Modelling, Validation, Adaptive Mesh Refinement, PA12*

Abstract:
One of the larger growing fields within additive manufacturing is the selective laser sintering process of semi-crystalline polymer powders. The powder particles are sintered together in local areas due the energy coming from a laser. This method allows for rapid manufacturing of complex parts, which are well suited for prototyping. The overall accuracy and stability of the process, along with part properties, are highly dependent on the involved process parameters. A better control of these parameters, will therefore lead to further optimization of the process. The current paper proposes a numerical modelling approach, for understanding the impact of major input parameters on the meso-scale thermal conditions, during the process. The model makes it possible, to analyze the influence of the laser-related input parameters, in relation to the temperature distribution and size of melt pool geometry, during the process. For validation, the predicted melt pool geometry is compared with the single-line track data found experimentally, where the melt pool geometry, can be compared to the numerical measurements by light optical microscopy and an in-situ infrared camera. Furthermore, an adaptive mesh refinement technique is developed and integrated in the model, which allows for modelling the thermal conditions of real-size parts within an acceptable computational time wtih a good agreement with experimental observations. The numerical approach is utilized through both costume code in Matlab, and by the commercial available software package COMSOL Multiphysics.

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Multi-scale Analysis for Microstructure Evolution in Powder Bed Fusion Process

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Key Words: *Powder Bed Fusion, Rapid Solidification, Non-equilibrium, Multi-phase filed Method, Lattice Boltzmann Method, Microstructure Evolution*

It is well known that microstructure in powder bed fusion process of additive manufacturing consists of grain and sub-grain, of which scales are 10-100μm and 0.1-1μm orders, respectively. This peculiarity is caused by its rapid solidification conditions of high cooling rate and high temperature gradient, 10^5-10^7K/s and 10^6-10^8K/m, respectively. Sub-grains in a grain have a common crystalline direction. Their boundary shows segregation of solidification. Consequently, numerical sub-grain microstructure evolution is considered to lead to prediction of mechanical property and design for heat treatment condition in this process.

In this study, a non-equilibrium multi-phase field method, based on finite dissipation model, coupled with CALPHAD database was developed for rapid solidification in a nine components system of an engineering Ni alloy **[1]**. Columnar solidification microstructure evolutions were performed at various set of cooling rate and temperature gradient under an interface velocity, 0.1m/s. It was showed that the sub-grain (cell) space decreased as the cooling rate increased. This tendency was more agreement with the experimental measurement than multi-phase filed method using local equilibrium condition in the solidified interface.

The previous heat condition for the sub-grain microstructure evolution is decided by process conditions, laser beam power, beam radius, traveling velocity, *etc*. A new numerical methodology of grain scale microstructure evolution in powder bed fusion process was proposed by coupling with three-dimensional multi-phase filed for melting and solidification, lattice Boltzmann phase field method for gas and liquid flows with free surface and thermal calculation with moving heat source. By using this method, melting of powder bed, flow in melt pool and grain scale solidification were simulated. Sub-grain microstructure evolutions were demonstrated at cooling conditions in different positions in melt pool by week coupling with the grain scale simulation.

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Multiscale Computational Model for Microscale Residual Stress and Dislcoation Dynamics in Addtively Manufactured 316L Stainless Steel

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Key Words: *Additive manufacturing, Crystal plasticity, 316L stainless steel, Residual stress, Dislocation dynamics*

In metal additive manufacturing (AM) process, large temperature gradient and repeated heating-cooling cycles induce residual stress in as-built parts, which may lead to distortion and even cracks. A computational framework is developed to study how microscale residual stresses form and evolve in AM parts, including a thermal-fluid flow model, a phase field model for grain growth and a crystal plasticity finite element model (CPFEM). The framework is calibrated and validated by comparing with experimental results of two 316L stainless steel samples fabricated by different sets of process parameters. The generation, evolution and distribution of residual stress at grain scale are investigated by simulations. In addition, a continuous dislocation dynamics model is incorporated. The thermal history and deformation of grains extracted from CPFEM simulations are applied to dislocation model to study the formation and evolution of the dislocation structure during AM process. This work provides insights into the formation and evolution of residual stress at grain scale, and helps to further understand the formation of dislocation networks in AM material.

Nanoparticle-enhanced absorptivity of copper during laser powder bed fusion

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Key Words: *Laser powder bed fusion, Copper absorptivity, In situ calorimetry, Nanoparticle decorated powder, Thermal models*

Laser powder bed fusion (LPBF) of pure copper for thermal and electrical applications is hampered by its low near-infrared absorptivity and high thermal diffusivity. These material properties make it very difficult to localize the thermal energy needed to produce high density 3D printed parts. Modification of metal powders via nanoparticle additives is a promising approach to increasing absorptivity, but the effect of nanoparticles on absorptivity and melting behavior during LPBF is not well understood. In this study, we developed an in situ calorimetry system to measure effective absorptivity during LPBF on copper substrates. We decorated copper substrates using three nanoparticle systems (CuS, TiB2, multilayer graphene flakes) and demonstrated an enhanced absorptivity of the decorated substrates relative to pure copper. Graphene nanoflakes resulted in the highest improved absorption relative to pure copper from 0.09 to 0.48, due to their stability at high laser scanning powers. A thermomechanical model with convective heat transfer provided confidence in the measurements by reproducing the experimental melt pool traces. Full 3D cylindrical prints demonstrated an improvement in relative density of the copper-graphene powder prints (in the range of 0.930–0.992), relative to that of as-purchased copper powder prints (in the range of 0.854–0.972). This work provides a fundamental study of nanoparticle-enabled LPBF of highly reflective metals and demonstrates a viable route for expanding the library of reliably printable metals. These results have been published in [1].

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Numerical and Experimental Analysis of Additively Manufactured Particle Dampers

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Key Words: *Additive Manufacturing, Particle damper, Laser powder bed fusion, Discrete element method.*

Particle damping is an effective passive method of vibration suppression. The remarkable advantages of particle damper, such as insensitivity to ambient temperature and availability at a wide range of frequencies, make it available for various applications [1]. However, a limitation for applying traditional particle damper is that an additional installation space is needed.

Additive manufacturing (AM), especially laser powder bed fusion (LPBF) technology, has been gradually adopted as an efficient method for fabricating multifunctional structures. By utilizing LPBF, a new integrated particle damper can be produced by deliberately leaving unfused powder inside the structure, named additively manufactured particle damper (AMPD). It has unique merits, such as neither mass nor cost is increased, and no additional space is required [2]. However, the damping mechanism and performance of AMPD are still unclear, more research is needed.

This research focuses on experimentally and numerically investigating the damping mechanism and performance of AMPD at a wide frequency range. A numerical simulation approach based on the discrete element method (DEM) was developed to predict the damping performance of a particle damper. To reduce the computational cost, a multi-unit particle damper (MUPD) was introduced, simulation model with only one unit cell was built A series of particle dampers of 316 L stainless steel with different numbers and sizes of unit cells were produced using LPBF. Experiments were carried out and compared with simulation results.

As a result, the numerical results of the proposed simulation model agreed well with experimental data, verifying that the proposed numerical method and simulation model are reasonable for analyzing the damping performance of additively manufactured multi-unit particle damper (AM-MUPD). The damping mechanism of AM-MUPD was clear by the numerical analysis. And the influence of different cavity numbers and sizes on the damping performance of AM-MUPDs was investigated experimentally.

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Numerical simulation of 3D laser surface melting and polishing processes

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Key Words: Coupled problems, Free surfaces, Incompressible flow with solidification, Marangoni effects, Operator splitting, Multi-grids, Laser surface melting

We present a multi-physics, multi-domain, model for the approximation of the coupled system formed by the temperature-dependent Navier-Stokes equations with free surfaces. The main applications are the industrial processes of shallow laser surface melting (SLSM), and laser polishing of thin surfaces. The goal is to simulate the effect of the free surface and the internal motion of the melting pool on the surface roughness during laser polishing.

We consider incompressible flow equations with solidification, by using a classical Boussinesq approximation. We add thermal effects with an enthalpy-based convection-diffusion heat equation, and we model the laser source through physically-consistent boundary conditions. We incorporate surface tension effects and Marangoni forces on the free surface to drive internal motion in the liquid metal.

The numerical method incorporates all the physical phenomena within an operator splitting strategy. Diffusion processes, such as heat diffusion, and the Stokes model are solved with a finite element method, while the transport phenomena are solved with a characteristics method. The volume-of-fluid approach is used to track the free surfaces between the (liquid or solidified) metal and the ambient air.

The numerical space discretization relies on a multi-grid, multi-domain, approach, relying on an unstructured finite element mesh and a structured Cartesian grid. Local mesh refinement is incorporated in order to accurately track the free surfaces. The multi-domain approach allows to solve the flow equations only in a neighborhood of the melting pool and the heat equation in a larger domain.

The numerical model is benchmark through some numerical experiments. In particular, we investigate the sensitivity of Marangoni effects and the influence of the free surface on the liquid metal during the re-melting process.

This is joint work Prof. M. Picasso, J. Hess (EPFL), and A. Masserey (Ycoor systems SA).

Phase-Field Simulation of Melting and Solidification of Al-Si Hypoeutectic Alloy under Conditions for Powder-Bed Fusion

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Key Words: *Additive manufacturing, segregation, Al-Si eutectic alloy, phase-field simulation*

Aluminum alloys are widely used for lightweight structures such as aerospace and automobiles owing to their low density. Further weight reduction is possible by utilizing topology optimization to minimize the volume of materials to achieve the required strength. Recently, additive manufacturing (AM) technologies have attracted much attention because they enable us to build complicated geometry 3-D parts with little difficulty. Moreover, the AM processes, in particular, powder bed fusion (PBF), can control material properties significantly via the control of solidification conditions and resultant microstructure, through the control of process parameter, such as power, diameter, and scanning speed of the laser beam. However, the relationship between solidification conditions and microstructures remains to be elucidated even for Al-Si alloys, which are commonly used in AM. In the previous study [1], the solidification of Al-Si alloys during PBF processes was simulated using the Multi-phase field (MPF) method, and only columnar crystalline grains appeared in the solidified microstructure. However, equiaxed crystalline grains were observed in the additively manufactured Al-Si alloy [2]. In this study, a heterogeneous nucleation mechanism was introduced to MPF simulation, and its effect on the solidification microstructure was investigated. In the actual PBF process, re-solidification occurs after the substrate is lowered by layer thickness. Therefore, the formation of re-solidified microstructures need to be investigated.

MPF simulation of an Al-10 mass % Si alloy was performed using microstructure evolution simulation software MICRESS for a region of 50 μm × 100 μm using a 50 × 100 grids domain with a one-dimensional temperature field. The system was cooled down with a cooling rate of 10^4 K/s. Then, the solidified model was re-melted at a heating rate of 10^4 K s^{-1}. After melting up to 75 μm of the material from the upper edge i.e., 75% of the simulation domain, the re-melted model was re-solidified at the cooling rate of 10^4 K s^{-1}, which is the same as the rate of the initial solidification.

In the simulation of solidification with heterogeneous nucleation, columnar α-Al crystals approximately 5 μm wide and elongated along the growth direction were formed. Then, eutectic regions comprised of α-Al and Si phases were formed between the dendritic columnar crystals and between their secondary arms. It is suggested that α-Al grains nucleated at the liquid/Si interface trigger further nucleation of Si crystal at the liquid/α-Al interface. The solidified Al-Si alloy model was heated until the melting of 75 μm from the upper edge. The solidified microstructure melted inhomogeneously: columnar dendrites of the α-Al phase were fully melted, whereas the regions of eutectic-microstructure were melted partially and the crystalline diamond-Si particles remained. Subsequently, in the re-solidification process, dendrites grew isotopically near the fusion line, and equiaxed grains of ~20 μm in diameter were formed.

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Phase-field study of precipitation from solute segregation in IN738LC Ni-based superalloy solidified under conditions for powder bed fusion additive manufacturing

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Key Words: *additive manufacturing, segregation, precipitation, superalloy, phase-field method*

Ni-based superalloys have been mainly produced by casting followed by solution treatment for homogenization of solute distribution and subsequent aging treatment for the precipitation hardening. On the other hand, additive manufacturing (AM) technologies are emerging as a new process for fabricating parts various materials including made of superalloys. Generally, rapid solidification is effective to avoid the solute segregation. Solidification by AM, in particular, powder bed fusion (PBF) process is characterized by the high cooling rate of around 1 million K/s. Such a rapid cooling is expected to result in a uniform solute distribution. It might allow the aging treatment without homogenization pre-treatment. However, resent studies have revealed the very fine submicron-sized cellular structures are formed in Ni-based superalloys fabricated by PBF process. Solute segregations between the cellular crystals are expected to affect the precipitation behaviour of gamma-prime phase.

In the present study, phase field simulations have been conducted to investigate the precipitation of γ'-phase from the solute concentration field generated by rapid solidification as initial condition. The multiphase-field method was applied to the simulation of microstructural evolution in directional solidification under various solidification conditions focusing on the solute segregation. A composition consisting of five major elements of Inconel738LC alloy, to which the application of AM is highly demanded, was selected as the model alloy composition. Gibbs free energies of liquid phases and FCC phase were evaluated by using thermodynamic database TCNI-9. The mobility database MOBNI5 were employed for the mobilities of elements. Initially, cellular structure with intercellular micro-segregation was generated by simulating directional solidification under a condition with cooling rate of 10^6 K/s, solidification rate of 10^{-1} m/s, temperature gradient of 10^7 K/m, which is a typical solidification condition in PBF process. Aluminium and titanium, which are γ' forming elements, segregated while other elements depleted at the intercellular region. In the subsequent aging at 1050°C, the growth of γ' precipitates and the relaxation of the segregation occurred simultaneously, and there was no significant influence of the segregation on the precipitates. In the case of aging at 850°C, aluminium depletion occurred at the intercellular region while titanium segregation remained before precipitation. The composition of the γ'-precipitates at the intercellular region are different from that in the intracellular regions. If the difference is negligible, the aging treatment without homogenization pre-treatment is applicable to the alloy fabricated by PBF. If the difference is not negligible, the segregation needs to be eliminated by solution treatment before ageing treatment. These results are to be validated by experimental analysis, and the values of parameters used tentatively are to be tuned so that the segregation predicted by this approach will be useful for optimizing AM process and designing novel alloys more suitable for AM process.

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Phase-field study of segregations in Ni-based superalloys solidified under conditions typical of powder bed fusion additive manufacturing

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Key Words: *Additive manufacturing, segregation, superalloy, phase-field simulation*

Superalloys are used for jet engines and gas turbine because of their excellent heat resistance and high-pressure resistance. Additive manufacturing (AM) is emerging as a new process for various materials including superalloys since it is expected not only to lower the costs by reducing the number of parts to be assembled but also to improve performance by controlling microstructures. Solidification microstructures formed by AM have characteristics different from those in cast counterparts, such as the absence of secondary dendrite arms, fine primary arm, and so on. For solidification of superalloys, it is important to control segregation as well as grain structure because it would cause cracking. The Scheil-Gulliver simulation is commonly used for predicting segregation in solidification under the imaginary extreme condition [1]. However, a more sophisticated method to predict the segregation taking the influences of the geometrical factors and kinetic factors is demanded. Phase-field method is suitable for this purpose. In the present study, the multiphase-field method was applied to the simulation of microstructural evolution in directional solidification under various solidification conditions with a special focus on the solute segregation.

Hastelloy-X was selected as the base of model alloys since it is one of the superalloys applicable to AM. Gibbs free energies of liquid phases and FCC phase were evaluated by using thermodynamic database TCNI-9. The mobility database MOBNI5 were employed for the mobilities of elements. For the mobility of solid/liquid phase change, the value for IN718 in a literature was used. Simulations were conducted under various solidification conditions in the range of $R = 10^{6}$~10^{-1} m/s and $G = 10^{3}$~10^{7} K/m with randomly orientated seed crystals finely distributed on the bottom edge of simulation box.

Geometrical grain selection occurred, and grains oriented to <100> in the solidification direction grew preferentially in all the cases. The widths of the columnar grains are comparable but larger than the experimentally observed one. The interdendritic segregation became more significant as the cooling rate increased, and was strongest for the case of the highest cooling rate of 10^{6} K/s ($R = 10^{-1}$ m/s, $G = 10^{7}$ K/m) which is a typical solidification condition in powder-bed fusion type AM process. The melting point for the composition of the interdendritic part with the segregation was much lower than that for the alloy composition, which would cause liquation cracking associated with residual stress in the AM process. Also, the composition was preferred for the precipitation of brittle intermetallic phases which need to be eliminated by solution treatment for after fabrication by AM process. These results are to be validated by experimental analysis, and the values of parameters used tentatively are to be tuned so that the segregation predicted by this approach will be useful for optimizing AM process and designing novel alloys more suitable for AM process.

This work was supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Materials Integration for revolutionary design system of structural materials” (Funding agency: JST) and partly by JSPS-KAKENHI.

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Physically based bead topology model coupled with electro-mechanical power source model applied for wire and arc additive manufacturing

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Key Words: *Wire and arc additive manufacturing, Young-Laplace equation, Bead topology, Electro-mechanical power source*

Metal additive manufacturing (MAM) has grown, in recent years, very strong interest in academic researches as well as industrial applications. Among MAM processes, wire and arc additive manufacturing (WAAM) became very popular through its advantages in manufacturing of medium and large-scale components [1].

The present work is carried out in the framework of the WAS project [2] which deals with WAAM process. The process relies on an automatized welding process in which a part is built by successively deposed metal bead.

We propose a physically based bead topology model using the equilibrium between the hydrostatic pressure and the capillarity force, under two-dimensional hypothesis. This equilibrium can be described by the Young-Laplace equation. The proposed model can also estimate a bead topology which is deposed on a complex support such as an inclined or a curved one. To do so, the Young equation is used to balance the forces at tri-phase point [3]. Moreover, a deposed melted metal volume is necessary for the bead topology model. By modelling a gas metal arc welding (GMAW) power source system [4], the volume can be estimated and be used as a physical parameter for the bead topology model. Combining the topology and the power source models, the coupling model allows to simulate the topology of a part made of deposed beads via WAAM. In addition to the modelling, experimental profiles of the beads are used to validate the model.

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Physics-based nozzle design for optimal liquid metal jetting via multiphase flow simulation

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Key Words: *Liquid metal jetting, multiphase flows, computational fluid dynamics, nozzle design.*

The Drop-on-Demand liquid metal jetting process is recognised as a relatively fast and affordable printing method for the 3D Additive Manufacturing industry. It is characterized by ejecting a sequence of droplets from a microfluidic nozzle attached to the end of a pump where the metal is molten and gets pushed down under pressure gradient, generated via magnetohydrodynamic or pneumatic forcing. Given the quality constraint of the final product, jetting speed is limited by the relaxation time of oscillating meniscus (liquid-gas interface) at the tip of the nozzle due to dynamic interplay between surface tension and the imposed pressure gradient. High-speed printing requires designing a nozzle that reduces the relaxation time without compromising the desired droplet size, shape, and speed. We present physics-based nozzle design rules to achieve high-throughput and stable jetting in drop-on-demand liquid metal 3D printing. The design rules are based on scaling laws that capture the change of meniscus oscillation relaxation time with geometric characteristics of the nozzle's inner profile. These characteristics include volume, cross-sectional area, and inner surface area of the nozzle. Using boundary layer theory for the simplified geometry, we show that the relaxation time of the meniscus is inversely proportional to the total inner surface area to the volume of the nozzle. High-fidelity multiphase flow simulations run in OpenFOAM verify this scaling. We use these laws to explore several design concepts with parameterized classes of shapes that reduce the meniscus relaxation time while preserving desired droplet specs. Finally, we show that for various nozzle profile concepts, the optimal performance can be achieved by increasing the ratio of the circumferential surface area to the bulk volume to the extent that is allowable by manufacturing constraints.

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Reduction of thermal distortion of laser powder bed fusion based on sequential inherent strain method

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Key Words: *Variable lattice density optimization, Powder bed fusion, Thermal distortion, Inherent strain method, Thermo-mechanical analysis*

Reduction of the thermal distortion caused by metal additive manufacturing's fabrication process is an important issue. Considering the problem of forming an object with lattice structures inside it to reduce the thermal distortion, we perform lattice density distribution optimization and experimental verification. Assuming a cube with a sphere void as the base lattice shape, the optimization problem is constructed based on the recurrent formula inherent method, the sensitivity analysis, and the method of moving asymptotes (MMA). The design variable is the representative size of the lattice geometry. The lattice's effective stiffness tensor is derived using the homogenization method, and the approximation function between the design variable and the effective properties is derived. The inherent strain value is calibrated using some test pieces with uniform lattice densities. Herein, the optimization is performed for quasi-two-dimensional and three-dimensional examples. Its experimental verification is finally performed by selective later melting fabrication and clearance measurement caused by warping deformation.

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Simulating Steering-Induced Defects in Composites Additive Manufacturing

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Key Words: *Process Simulation, Composites, Automated Fibre Placement, Defects*

Additive manufacturing techniques for composites, such as automated tape laying (ATL) and automated fibre placement (AFP) have become more mainstream in the aerospace industry over the last 20 years. These techniques rely on the use of a computer-aided machine which places the composite prepreg layer-by-layer according to the part geometry and layup design. It has been shown that these methods allow reduced waste and improved work efficiency with an overall 70 to 85% reduction of the layup time. However, one of their key limitations is the generation of manufacture-induced defects that can result in up to 35% degradation of the structural performance of the finished part. With the increasing complexity and size of structures in which composites are used, the traditional trial-and-error approach to mitigate these defects becomes extremely costly. This explain the recent increase in scientific publications aiming at modelling and simulating the ATL/AFP deposition process, with a view to replacing the large numbers of physical trials that manufacturing process development currently requires.

However, in many cases, current state of the art simulation is limited to one single value for each process parameters. This is, in part, due to lack of constitutive models able to capture the complex mechanical behaviour of composite prepregs that show viscoelastic features and strongly depends on temperature and deformation rate. In the present contribution, a multi-body modelling platform of the AFP process is presented. Previous work on characterisation and modelling of composite prepregs [1,2] forms one of the building blocks of the current framework, which is shown to be able to capture final tape quality resulting from different combinations of temperature and deformation rate. This paper gives further insights into the understanding of automated manufacturing of composites and lays the ground for process optimization, defect mitigation and overall improvement of part quality.

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Simulation of keyhole dynamics and keyhole pore formation during metal additive manufacturing

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Key Words: Keyhole pore, Additive manufacturing, Multiphysics thermal-fluid flow model, Molten pool flow, Low ambient pressure

Metal additive manufacturing has gained extensive attention from research institutes and companies to fabricate intricate parts and functionally graded materials. However, the porosity of the as-built part deteriorates the mechanical property and even hinders the further application of metal additive manufacturing. Particularly, the mechanisms of keyhole pores associated with the keyhole fluctuation are not fully understood. To reveal the mechanisms of the keyhole pores formation, we developed a multiphysics thermal-fluid flow model [1, 2] incorporating heat transfer, liquid flow, metal evaporation, Marangoni effect, and Darcy's law to simulate the keyhole dynamics and keyhole pore formation process, and the results are validated with the in-situ X-ray images.

The geometry features of the simulated keyhole and melting pool showed a good agreement with the experimental observation by ultrahigh-speed X-ray imaging in Argonne National Lab. To understand the physical mechanisms of keyhole fluctuation, the laser energy distribution on the keyhole surface, and the driving forces on the keyhole surface were further analyzed.

The simulation results present the keyhole pore formation stages: instant bubble formation due to the keyhole instability and motion of the instant bubble when it pins on the solidification front. The simulation results indicate that the unevenly distributed recoil pressure on the keyhole surface is an important factor for keyhole collapse and penetration. Furthermore, comparing the keyhole pore formation under different laser scanning speeds shows that the keyhole pore is sensitive to the manufacturing parameters. The keyhole fluctuation features and energy absorptivity variation on the rear keyhole wall could be metrics to evaluate the likelihood of the keyhole pore formation.

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Space-time formulation for heat evolution in laser based powder bed fusion

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Key Words: *heat evolution, space-time, melt pool shapes, validation*

The direct numerical simulation of metal additive manufacturing processes such as laser-based powder bed fusion of metals (PBF-LB/M) is challenging due to the vast differences in spatial and temporal scales. Classical approaches based on locally refined finite elements combined with time-stepping schemes can only address the spatial multi-scale nature and provide only limited scaling potential for massively parallel computations. We address these shortcomings in a space-time Galerkin framework where the finite element interpolation also includes the temporal direction. In this setting, we construct four-dimensional meshes that are locally refined towards the laser spot and allow for varying temporal accuracy depending on the position in space. By splitting the mesh into conforming time slabs, we recover a stepwise solution to solve the space-time problem locally in time at this slab; additionally, we can choose time-slab sizes significantly larger than classical time-stepping schemes. We use a continuous Galerkin-Petrov formulation of the nonlinear heat equation with an apparent heat capacity model to account for the phase change [1].

We validate our approach by computing the AMB2018-02 benchmark, where we obtain an excellent agreement with the measured melt pool shape. Further, we explore the range of validity of the approach by computing a range of Gaussian to doughnut shaped laser profiles by calibrating only towards one setting and checking the computational results against corresponding experiments [2]. This systematic study gives insight to when the convection based model turns invalid.

Finally, we apply the findings to a patch level and give an outlook on upscaling the computational model which offers the possibility for time and space parallel computations of heat evolutions in laser-based powder bed fusion processes.

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Synthetic Volume with Statistical Copy of Additive Manufactured Sample for 3D Crystal Plasticity Simulations

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Key Words: *Selective Laser Melting, Digital Twinning, Crystal Plasticity Simulations*

Crystal plasticity (CP) simulation of selective laser melting (SLM) metal materials is a challenge due to typically very complex shape and size of various anisotropically distributed chemical/microstructure phases governed by laser heat gradients and scanning patterns. Even image segmentation of such phases is a nontrivial but important task for structure/property relation analysis [1,2]. To conduct accurately the CP simulations of material's mechanical properties, the sophisticated synthetic volume (SV) reconstruction is required. An example of complete workflow pipeline for tensile test CP simulations with statistically accurate distributions of necessary parameters in SV from SEM and EBSD data will be presented for SLM samples of Inconel 738LC. The data pipeline and simulations were mainly conducted with Dream3D and DAMASK open-source packages [3,4].

In SV reconstruction, the statistical distributions of microstructure object sizes for each phase, several shape parameters for each microstructure type, and grain crystallographic orientations were taken into account. Each step in the pipeline, including parameters for CP modelling, can be fine-tuned to achieve suitable correspondence between experimental and simulated results. Then, various 3D stress/strain maps (equivalent von Mises stress/strain, et. cet.) could be hopefully used to locate/analyse the possible mechanical damage initiation centres and explained by comparing with grain crystal orientation and Schmid's factor maps.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Computational Inverse Design of Turing Pattern Inflatable Structures

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Key Words: deployable structures, shell element, orientation optimization, Turing pattern, 4D printing

Recently, programmed 3D shape or 4D printing is emerging as a new paradigm in additive manufacturing and receiving much attention since it provides printed structures with the ability to transform into various shapes or to alternate functions or stiffness over time according to environmental stimuli.

This study focuses on a computational design method for shape-morphing inflatable structures for 4D printing. Inflatable structures can easily change their shapes into 3D surfaces with a simple pressure input. These inflatable structures have been employed in science and engineering to enable the design of physical systems in diverse fields, including soft robots, airbags, and temporary shelters.

The present study addresses the programming of inflatable structures by designing the distribution of material orientations of their surface membrane. By prescribing the orientations, we can program the local deformation of the material and thus control their global shapes. For this purpose, we integrate a full physical simulation of the inflatable structures using the nonlinear shell finite element method in the inner loop of a gradient-based optimization algorithm that continuously modifies the distribution of the material orientations to improve design objectives. The material orientation in this optimization is a locally varying axial distribution where an orthotropic elastic material model including orientation tensor in its constitutive equation is utilized. The anisotropic membranes with the optimized distribution of the material orientations are fabricated by digital light processing (DLP) 3D printing[1]. Each pixel in the 3D printing, however, is limited to isotropic material. Therefore, the distribution of anisotropy is converted to a discretized texture pattern that induces an anisotropic deformation of the surface membrane. The anisotropic reaction-diffusion equations are then utilized to generate the space-filling discretized Turing pattern texture. Anisotropic diffusion coefficients in the reaction-diffusion equations are determined using the orientation tensors derived from the orientation optimization. The present method directly produces fabrication instruction or CAD data of the anisotropic materials.

In this contribution, several examples of the optimized shape-morphing inflatable structures are provided to illustrate the performance of the proposed design method.

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Enhancing Flexural Properties of Additively Manufactured AlSi10Mg Triply Periodic Minimal Surface Latticed Beams through Functional Gradation and Hybridization

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Key Words: *Cellular structures, Four-point bend flexural properties, Functional gradation, Hybridization, Triply periodic minimal surface.*

Abstract: Lattices produced through additive manufacturing are gaining momentum in bio-inspired material science research for designing lightweight and high-strength meta-materials for various engineering applications. Among many categories of well-ordered porous architectures, the mathematically-derived sheet-based triply periodic minimal surface (TPMS) porous structures are perceived to yield superior mechanical functionality due to their ease-to-manipulate topological features, stretching-dominated deformation mode, and uniform stress distribution capabilities [1, 2]. This paper aims to evaluate the influence of relative density grading and hybridization on the quasi-static four-point bend (4PB) flexural properties of AlSi10Mg sheet-based TPMS latticed beams fabricated through the laser powder-bed fusion process. 4PB elastic-plastic simulations are performed to compare with the experimental findings. Sheet-based TPMS porous architectures such as the f-rhombic dodecahedron (FRD), primitive (P), and diamond (D) with an average relative density of 20% and 4PB specimens with tessellation of $12\times4\times4$ unit-cells are considered in this work, based on the preliminary investigation on the effective elastic properties of the sheet-based TPMS cubic lattices. Generally, the specific flexural stress-strain curves obtained from the 4PB simulations agreed well with experiments, and the equivalent plastic strain contour plots showed to reliably predict possible failure trajectories per experimental observations of the 4PB sheet-based TPMS latticed beams. Specifically, varying the through-thickness relative density of the 4PB sheet-based TPMS latticed beams, e.g., bilinearly, the final failure of the specimen is retarded due to deflection of the propagated cracks in-contrast to observations made with the uniform specimens. Also, relative density gradation improved the specific flexural strength of the sheet-based TPMS latticed beams. Hybridization of the sheet-based TPMS latticed beams is inspired by the constant bending moment region in the load-span of the 4PB beam specimens and results reveal an improvement in the specific flexural stiffness (using the P-D-FRD-D-P configuration). More importantly, hybridization mitigated shear-band failure through which the uniform and relative density graded specimens failed.

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Parametric Visco-Hyperelastic Constitutive Modeling of Functionally Graded Polymers Manufactured via Grayscale Masked Stereolithography

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Key Words: Additive manufacturing, stereolithography, visco-hyperelasticity, functionally graded materials, photopolymerization, 3D printing

Grayscale masked stereolithography (MSLA) 3D printing enables the fabrication of graded structures from a single material, overcoming the limitation of vat-photopolymerization methods to a single material. Two main parameters affecting the curing of the resin in the stereolithography manufacturing method are the exposure time per layer and the intensity of the ultraviolet (UV) light in terms of the grayscale value of the mask, which have a significant influence on the resulting material properties. In our earlier work, the dependency of the resulting material properties on the parameters of the grayscale MSLA process was investigated and a grayscale-dependent hyperelastic material model was formulated [1]. Here, the concept of grayscale MSLA is extended by combining the two easily adjustable parameters exposure time and grayscale value into a single parameter, which we call the grayscale exposure. The advantage of expressing the degree of cure in terms of grayscale exposure is not only the reduction of design parameters from two to one, but also the fact that the printing time can be reduced through correlation of exposure time and grayscale. Then, a parametric visco-hyperelastic constitutive model is formulated for the strain rate-dependent behavior of the resulting material in finite deformations, which depends on the grayscale exposure. Hyperbolic tangent functions are utilized to express the material constants for different grayscale exposure. Furthermore, the grayscale exposure values are verified through a comparison of different couples of grayscale and exposure time. Finally, the constitutive model is validated with further experiments, showing a good agreement with experimental results.

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Two-way shape memory effect in semicrystalline networks: from modeling to 4D printing

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Key Words: Shape memory polymers, Two-way shape memory effect, Constitutive model, 4D printing

Soft materials capable of autonomously changing their shape with an on-demand and reversible response are considered very interesting in the fields of soft actuators and robotics [1]. To this aim, thermally-triggered two-way shape memory polymers possess two promising features, known as one-way and two-way shape memory effect (SME). The one-way SME is a non-reversible feature, describing the ability of the material to recover its original "permanent" shape from a deformed "temporary" one when heated. Contrarily, the two-way SME is a reversible feature, representing material capability to reversibly switch between two distinguished configurations under repeated cooling-heating cycles.
The present work proposes a new phenomenological constitutive model to describe the one-way SME and the two-way SME under stress-driven and stress-free conditions in semicrystalline networks, starting from the formulation presented in [2]. Specifically, we focus on the synthesis and characterization of semicrystalline networks based on poly(ε-caprolactone) crosslinked by a sol-gel approach or by photocrosslinking. Experimental results are used to formulate, calibrate, and validate the model. The proposed model is shown to be useful for the design and development of autonomous actuation systems. To this purpose, the effect of the macromolecular architecture and the employed thermo-mechanical parameters is investigated. Preliminary results concerning the additive manufacturing of these systems as well as the actuation of metamaterial structures will be presented and discussed.

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Macroscopic modelling and simulation of powder bed-based additive manufacturing of polymers

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Key Words: Simulation, Selective Laser Sintering, Polymers, Crystallization

In powder bed-based additive manufacturing (AM) complex part geometries can be built in a layer-by-layer fashion using locally restricted melting of powdered material. For Selective Laser Sintering (SLS) of polymers this is achieved in a process that can be grouped into three stages: (i) the pre-heating stage where the build chamber is heated up to a desired process temperature, (ii) successive layer deposition and melting and (iii) the cooling stage. The melting is accomplished by means of the energy provided by a laser beam. Further, in contrast to powder bed-based AM of metals, solidification of the molten material occurs not immediately after melting. Molten and powder material rest side by side after the melting process. Throughout the process, non-isothermal crystallization activities are then responsible for solidification which can occur not only in stage (iii) but also during the second process stage as shown e.g. in [2]. In order to model this behaviour a Nakamura model for crystallization is extended to allow for a re-melting as it occurs in SLS [3] and integrated into a verified and validated numerical tool [2]. Since macroscopic modelling and simulation of these manufacturing processes can rapidly lead to computational expensive models, adaptivity in both the spatial and temporal regime are necessary to reduce the potentially high computational cost [1]. This includes the possibility of sub-time stepping, i.e. the separation of the temporal integration domain and corresponding fields into regions that may be integrated with different time-step sizes. This allows to employ small time-step sizes only where they are needed [3]. Further, a thermo-mechanical coupling approach is used for the prediction of the temperature, crystallization and displacement fields on a macroscopic scale.

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Part-scale Thermo-mechanical Modelling for The Transfusion Module in The Selective Thermoplastic Electrophotographic Process

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Key Words: *thermo-mechanical model, part-scale model, flash heating, selective thermoplastic electrophotographic process*

Additive manufacturing (AM) is a breakthrough approach to industries, potentially relieving the limitation when producing complex geometries with traditional manufacturing processes. Selective thermoplastic electrophotographic process (STEP) is a brand-new AM process proposed by Evolve additive solutions Inc Solutions, Inc. The STEP process works based on layer-wise manufacturing by fusing 2D layers produced by electrophotography onto a 3D bulk structure. The principle of the 2D to 3D deposition process in STEP is through heating up both the incoming 2D layer and the bulk material and then applying pressure to fuse the 2D layer onto the already-built component. This deposition module in STEP is known as transfusion. With the two core modules, electrophotographic, and transfusion, STEP could create a fully dense and multi-material part [1], and the developers hope, it could be an alternative to injection molding.
In the present work we develop the first numerical model for the STEP process. It is a part-scale thermo-mechanical finite element model based on the flash heating (FH) [2] method in the commercial software package ABAQUS. FH is a part-scale method, originally developed to solve thermal problems in laser-based AM processes, without truly resolving the interaction between the heat source and the bulk material, but instead uniformly distributing the input energy on the recently-activated meta-layer. Both the part material, as well as the support material in the STEP machine are considered. The thermal and mechanical predictions are compared with relevant experimental measurements for validation purposes. A comprehensive manufacturing parametric study is also presented. This modelling approach will potentially pave the way for making a robust digital twin of the STEP process, that later could be integrated in the STEP process itself, serving as a feedback source for real-time correction of the input process parameters for achieving a close to defect-free end-product.

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Probabilistic Homogenization Analysis Considering Random Field of Microstructure in Resin Specimen Fabricated by FDM Method

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Key Words: *Probabilistic Analysis, Additive Manufacturing, Fused Deposition Modelling Method, Random Field, Autocorrelation, Monte-Carlo Simulation.*

Additive Manufacturing (AM) technology is very attractive forming approach for fabricating products by laminating molten materials. Currently, AM technology is being used not only in the industrial filed but also in various fields such as the medical field based on various research and development activities. However, since it is difficult to control the fabricating process perfectly comparing to conventional existing forming methods, complexity and randomness in the mechanical properties and shape will be observed in the products. In particular, Fused Deposition Modelling (FDM) Method used in this study is a method of creating components by laminating molten resin under small pressure, which will result in a heterogeneous microstructure. Geometrical randomness in this heterogeneous microstructure will have an influence on the apparent mechanical properties, and therefore, it is necessary to be considered in design of such products.

For this problem, the results of stochastic homogenization analysis of components fabricated by FDM method have been reported[1]. Also, in response to this result, the results of an analysis using a model that considers the random field (RF) of the microstructure have been reported[2]. However, in this report, the RF of the microstructure considers the RF inside a certain specimen. In fact, the spatial autocorrelation, mean and standard deviation in the RF will be different from them of each specimen, so they need to be considered.

In this study, multiscale probability analysis considering a difference of probabilistic property in each specimen. Specifically, RF using the moving window method[3], Monte Carlo (MC) simulation, and multiscale stochastic analysis based on the homogenization method were used to calculate the apparent elastic modulus and compare it with the experiment to investigate the effect of considering the RF of each specimen.

In this presentation, a procedure for creating an analytical model that considers the characteristics of the RF obtained from specimen observation is introduced, and numerical results are shown for discussion on the effectiveness of considering RF for each specimen.

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Accelerated constrained shape optimization

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Key Words: Constrained shape optimization, gradient-based optimization, Nesterov's Accelerated Gradient

High-fidelity shape optimization based on Finite Element mesh is inherent large-scale, in which millions of design variables may be considered in industrial applications. Gradient-based optimization is almost the only viable solution strategy. In many practical circumstances, a number of constraints need to be considered, such as cost, material limits, manufacturability, and usability. Needless to say, it is a genuine engineering work how practical constraints can be modeled so that a gradient-based optimization can be applied. Motivated by these applications and inspired by singular value decomposition, a gradient descent akin method (GDAM) has been developed for solving constrained optimization problems. At each iteration, a search direction is computed using a linear combination of the negative and normalized objective and constraint gradient. While the principled idea behind GDAM is similar to that of gradient descent, we show its connection to the classical logarithmic barrier method and argue that it may be considered a first-order interior-point method. Vanilla implementation of GDAM has demonstrated its potential in solving large-scale shape optimization problems. However, a large number of iterations may still be needed for difficult problems. In this work, we present an accelerated version of GDAM for constrained shape optimizations based on Nesterov's Accelerated Gradient (NAG). NAG is an optimal method in terms of oracle complexity for unconstrained minimizations. Its convergence rate $o(1/k^2)$, with k as the iteration number, excels the gradient descent method with a rate of $o(1/k)$. In this contribution, we present an implementation how NAG can be applied to GDAM (denoted as GDAM + NAG) and show computational results. In common benchmark tests, GDAM + NAG achieves 10x faster convergence rate compared to GDAM. Finally, we show a large-scale constrained shape optimization, where the iteration number is reduced from approx. 200 to 20. Our results strongly suggest the practical relevance of the present algorithm.

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Adaptive Vertex Morphing parameterization for large node-based shape optimization problems

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Key Words: CAD-Free parameterization, Adaptive Vertex Morphing, Shape Optimization, Relaxed Gradient Projection

There are various methods to parameterize the design space for large shape optimization problems. One of them is Vertex Morphing (VM) [1]. It is a node-based shape parameterization technique that directly uses the surface nodes of the Finite Element model as a design parameters. Vertex morphing filters the shape update and sensitivities to keep the design surface smooth and continuous. Nowadays, the Vertex Morphing technique is a successful shape parameterization technique used in academia and industry. [2] [3]

In our work, we present an extended version of Vertex Morphing, "Adaptive Vertex Morphing" (AVM). The main idea of the AVM method is to separate two roles of the filtering radius and extend the design possibility of Vertex Morphing parameterization. On the one hand, the radius should be sufficiently big to filter sensitivities and generate smooth shape updates. On the other hand, the size of the radius is an additional design parameter, which controls the final design. Adaptive Vertex Morphing computes respective radii for each node every optimization iteration, based on the local mesh size, to ensure that the filtering is successful during the optimization process. Additionally, a user can set up local or global radius values to "constraint" the shape update modes to a specific wavelength and better control the final design.

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Adjoint-Based Shape Optimization for Industrial Heat Exchangers

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Key Words: *Multiphysics Problems, CHT, Discrete Adjoint, Industrial Applications*

Power electronics as used in electric cars derate their performance above certain temperatures, if not sufficiently cooled. Residential gas/hydrogen boilers require careful design for optimal efficiency and minimal emissions. In both application fields, a free-shape optimized design of the heat exchanger and surrounding components promises substantial performance gains that are relevant to fulfil the regulator's and customer demands.

The discrete adjoint method using automatic differentiation to compute shape gradients for CHT problems [1] will be outlined together with an efficient way to evaluate a pin-shape performance, essential in many heat exchangers, using streamwise periodic flow. Validation of the discrete adjoint gradient against finite differences shows excellent agreement for all tested configurations. These sensitivities are used in a shape optimization process using FFD-boxes and competing objective functions (system pressure drop and surface temperature or similar). Beyond shape optimization, the value of accurate shape sensitivities on its own for industry will be highlighted, as suitable shape parameterization with an effective enforcement of geometry constraints are not a trivial step.

In addition to the results of steady state simulations, validated gradients for a simple unsteady CHT setup using the discrete adjoint method are implemented and available. The unsteady multizone adjoint requires additional care [2] in terms of implementation and especially objective function definition.

The implementations that were used to produce the results are available to the public via the open-source C++ code SU2 [3]. The contributions are embedded in a code framework that encourages collaboration between academia and industry to extend features and usability.

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Aerodynamic and Acoustic Design Optimization of a Multiple Propeller Combination for Distributed Electrical Propulsion

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Key Words: *Distributed Electrical Propulsion, High-Lift, Multiphysics Problems, Multi-Point Design, Evolutionary Computing*

This work aims at optimizing a large-scale wind tunnel model conceived to investigate the aerodynamic and acoustic performance of distributed electrical propulsion (DEP) on aircraft wings in high lift conditions. The aim of the optimization process is to obtain the best possible improvements in Noise and Aerodynamic performance by modifying the propellers' layout of the Wing-DEP wind tunnel model. A multi-objective, multi-point design approach is adopted based on evolutionary computing. The robustness of the obtained solution set is also investigated. The research work is carried out in the framework of VENUS EU-funded project GA N. 886019.

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Basic Examinations of Non-parametric Shape Optimization Problems and their Applications to Real-World Problems

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Key Words: Shape Optimization, Topology optimization, Function Space, Fréchet Derivative, Gradient Method, Newton Method

In this talk, the "Large-scale problems" in the scope of the minisymposium "Shape Optimization for Large-Scale Problems" is involved in the definition of design variables using functions, which formulations are referred as distributed parameter systems or non-parametric systems. Since the degrees of freedom of the functions are infinity, there is a possibility which becomes "Large-scale problems".

The target problems discussed in this talk are topology optimization problems of density variation type and shape optimization problems of domain variation type. The key point in the formulations is how to select the vector spaces for the design variables. Thanks to the functional analysis, we can define appropriate function spaces for the two types of problems, and evaluate the Fréchet derivatives of cost functions with respective to arbitrary variations of the design variables. To solve the problems, we can consider gradient methods and Newton methods defined in the function spaces of the design variables[1].

The aim of this talk is to introduce the aforementioned theories briefly, and shows the results of the basic examinations using computer programs developed by means of a programing language by the finite element method, FreeFEM. Especially, how the convergence phenomena reflect the theoretical results regarding regularity of boundary in the numerical results is discussed using concrete problems.

In addition, the applicability of these optimization frameworks to real-world problems are then illustrated through several examples that were due to the students and researchers from the presenter's laboratory.

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Data-Driven Analysis, Design, and Optimization in Fluids Engineering

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Key Words: Fluids Engineering, Data Science, Bayesian Optimization, Surrogate Modeling, Shape Optimization, Topology Optimization

Fluids engineering involves complex nonlinear physics due to viscosity, shock wave, turbulence, etc. It is essential but costly to analyze the physics of fluids for engineering applications, such as vehicle and turbomachinery. Nowadays, data science is expected to leverage practical applications of fluids engineering for various purposes, mainly design and optimization.

Design and optimization ask designers to analyze many design candidates to be evaluated, one of which is expected to be optimal. Data science can replace expensive analysis with an inexpensive estimation of the quality of interest (*e.g.*, performance) for any unknown design candidate based on the database available for the existing design candidates. Hence, design science helps the designers to find the optimal design candidate efficiently. However, the inexpensive estimation based on data science may disagree with true evaluation by expensive analysis, which affects the fidelity of the optimized design.

Our research group has been working on Bayesian optimization, which aims to find the optimal design under uncertainty in the estimation based on data science in a data-driven way, as an effective analysis and design tool. Bayesian optimization is promising to balance exploration and exploitation, i.e., fidelity and quality of the optimal design within a realistic database size.

This talk will present our original learning-based surrogate modeling, which can model any nonlinear response in the quality of interest to be estimated for Bayesian optimization [1]. Moreover, this talk will present some applications of Bayesian optimization to real-world design, *e.g.*, shape optimization of a low-boom supersonic transport [2] and topology optimization of a lattice-structured heat sink [3].

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Discrete Adjoints for Multiphysics Problems

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Key Words: Discrete Adjoints, Multiphysics, MDO, Algorithmic Differentiation, Shape Optimization

The discrete adjoint approach to design offers a computationally inexpensive and precise way to obtain sensitivity information for optimization problems in Computational Fluid Dynamics [1] and related fields. For partitioned multiphysics problems, like fluid-structure interaction, conjugate heat transfer or even more complex combinations of different kinds of physics [2], the gradient of an objective function with respect to design parameters can analogously be derived from *coupled* discrete adjoint solutions, computed for each sub-discipline. The difficulty is, however, to capture and include their adjoint coupling terms, so-called cross derivatives or cross terms, that originate from the exchange of solution data between solvers during the primal simulation process.
In this talk, we will present a methodology [3] whereby adjoint solutions can be computed efficiently and in a way that is completely independent of the underlying physical sub-problems, the associated numerical solution methods, and the number and type of couplings between them. Furthermore, by applying the reverse mode of algorithmic differentiation to each discipline, and by using a specialized recording strategy, diagonal terms and cross terms can be evaluated individually, thereby allowing different solution methods for the generic coupled problem (for example block-Jacobi or block-Gauss-Seidel).
On the basis of an implementation in the open-source multiphysics simulation and design software SU2 [4], we demonstrate how the same algorithm can be applied for shape sensitivity analysis on multiphysics problems coming from heat transport (a pin-fin heat exchanger), from aerodynamics (a wing that deforms under flow tractions) or from propulsion (a turbine blade in high-temperature flow).

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Higher-Order Shape Optimization Based on Variational Derivatives

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Key Words: Variational Shape Hessians, Adjoints and Material Derivatives, Shape Newton Schemes

A variational approach for higher order shape optimization based on the distributed formulation of the shape derivative is considered. Within this approach, the adjoint is used to eliminate material derivatives instead of partial derivatives, which leads to a very convenient way to derive a Newton scheme for shape optimization. In particular, this approach also allows an interpretation of the Sobolev gradient descent methods as an approximation of the shape Hessian when the perimeter is used as a regularizer.

The methodology quite naturally leads to a variational formulation to compute the 2nd order shape updates and opens the door to novel numerical schemes, not only in classical aerodynamic shape optimization, but also to construct particularly fast solvers for free surface flows and microfluids.

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Large-Scale Industrial Shape Optimization Applications in Maritime Two-Phase Flows –Learning from the Adjoint–

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Key Words: Adjoint-Based Shape Optimization, Computational Turbulent Maritime Two-Phase Flow

The presentation outlines strategies to advance gradient-based optimization methods based upon the continuous adjoint approach for CAD-free (non-parametrized) marine engineering shapes which are exposed to immiscible two-phase flows at very large Reynolds ($Re>10^8$) and Froude number ($Fn>0.35$). Issues addressed refer to the relevance of adjoint consistency, the preservation of industrial process capability and the computation of geometrically constraint shape gradients in compliance with the deformation of the mesh. It is seen that potential weaknesses revealed by an adjoint approach, e.g. when aiming at the development of closed analytical solutions or in conjunction with convergence problems, are often attributable to weaknesses of the primal flow model. To this end, a twist of the research question can lead to fruitful insights, which can significantly improve the numerical robustness and the accuracy of large scale practical applications. Contributions refer to the development of an efficient engineering Cahn-Hilliard (CH) Volume-of-Fluid (VoF) branch [1]. In line with analytical considerations for a model problem, a nonlinear Equation of State (EoS) is derived to relate an indicator function with the fluid properties. This allows for a robust and consistent adjoint two-phase formulation [2]. A second focus is put to improving adjoint turbulent flow models using mixing-length arguments to replace the frozen turbulence strategy [3] by an algebraic expression derived from the adjoint momentum equation in the logarithmic layer. Thirdly, an implicit surface metric approach is presented to simultaneously extract an inherently smooth shape gradient and mesh deformation from the same procedure. Moreover, attention is devoted to the compliance of the shape update with local and global geometrical constraints, i.e. constant volume or maximum outer dimensions. Finally, an adaptive floatation module is added to the gradient-based optimization procedure. Applications relate to maritime two-phase flows at the industrial level in full-scale.

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Structural optimization in ANSYS

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Key Words: *Level-Set Method, Shape and Topology Optimization, Shape Sensitivity Analysis*

In 2019, ANSYS was the first software editor to deliver level-set based Topology Optimization (TO) [1]. This disruptive technology facilitates both the formulation and handling of several manufacturing and mechanical criteria that are commonly used in industry, thus expanding the applicability of TO for real-world applications. ANSYS is also delivering a real-time topology optimization engine based on GPU computing [3] that fits for early stage of the conception cycle when it comes to quickly sketch designs or explore different scenarios.

The watertight level-set description offers several advantages:
- Formulation of independent geometric criteria without relying on complicated filtering techniques. This is advantageous when several constraints need to be applied simultaneously to account for manufacturability: Minimum and Maximum Member Size, Pull-Out, Overhang, Center of Gravity, Moment of Inertia, Volume, etc.
- Requires no dedicated treatment in the construction of material interpolation schemes or the formulation of mechanical constraints such as eigenfrequencies, stress etc., which allows to combine them efficiently in the formulation of the optimization problem.
- Post-treatment of the TO results under minimal effort and maximal fidelity. Using SpaceClaim of ANSYS, the back-to-CAD process is user-friendly and nearly instantaneous, saving significant amount of work for the user. At the same time, since no interpretation step of densities is needed, the design validation process becomes quite straightforward.

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Real-time Bead-on-Plate weld Simulation for Wire Arc Additive Manufacturing using Reduced Order modelling coupled with stochastic model Calibration

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Key Words: *wire arc additive manufacturing, reduced order modelling, model calibration*

Numerical simulations are essential in predicting the behavior of systems in many engineering fields and industrial sectors. The development of accurate virtual representations of actual physical products or processes (also known as digital twins) allows huge savings in cost and resources. In fact, digital twins would allow reducing the number of real, physical prototypes, tests, and experiments, thus also increasing the sustainability of production processes and products' lifetime. Standard numerical methods fail in providing real time simulations, especially for complex processes such as additive manufacturing applications.

This work aims to use a reduced order model for efficient wire arc additive manufacturing simulations, calibrations and real-time process control. Model reduction, e.g. the proper generalized decomposition [1,2] method, is a popular concept to decrease the computational effort. A new mapping approach [3] was applied to simulate a moving heat source with the proper generalized decomposition. Using this procedure even complex models can be simulated in real-time. The physical model is later on calibrated with the use of a stochastic model updating process and the reduced order model, leading to an optimized real-time simulation.

In this contribution, a proper generalized decomposition model for a bead-on-plate wire arc additive manufacturing is presented. It is also coupled with a stochastic model updating process identifying the heat source characteristics as well as the boundary conditions of the transient thermal problem, whereas the heat source shape is simulated using a Goldak heat source [4].

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Towards Part-Scale Simulation of Metal Additive Manufacturing

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Key Words: Metal Additive Manufacturing, Part-Scale Simulation, Model Hierarchie

The strongly localized energy input prevalent in many metal additive manufacturing (AM) processes gives rise to large thermal distortions as well as high residual stresses, which in combination with residual porosity might even induce cracking of the part already during the production process. While predictive thermomechanical models would be highly desirable for systematic process and geometry optimization, the inherent multi-scale nature of these processes still prohibits part-scale simulations with geometrically resolved heat source path. Apart from computational efficiency, also the aspect of constitutive modeling, taking into account the strongly inhomogeneous and anisotropic evolution of microstructure and resulting material properties during the process, is critical for an accurate residual stress prediction.

In [1], the authors proposed a thermomechanical model for metal AM processes, in which the boundaries between powder, melt and solid phase are described as diffuse interfaces. The underlying constitutive law, derived via Voigt-type spatial homogenization, incorporates a reference strain term in rate form that allows to consistently represent a stress-free state for newly solidifying material at melt temperature. In our talk we will present strategies to formulate models of different detailedness on basis of this material law. It will be demonstrated how the resulting hierarchical modeling framework, embedded in a parallel code platform, can be employed to foster computationally efficient simulations on part-scale.

A second focus of the talk will lie on coupled microstructure and material modeling. In [2], a physics-based and data-supported microstructure model for Ti-6Al-4V has been proposed, which predicts metallurgical phase fractions in a continuum sense instead of resolving individual crystal structures. In our talk we will present a general procedure to utilize this computationally efficient microstructure model for thermomechanical part-scale simulations based on microstructure-informed material laws.

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Full-scale reconstruction of kinematically enhanced constitutive modelling approach

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Key Words: *Consolidation, Process-Modelling, Kinematic enrichment, Variability*

Out of tolerance thickness variations and fibre path defects are a reccurring issue in thick tapered laminates, resulting in a knock-down in mechanical properties and potentially preventing composite manufacturing processes from becoming commercially viable. The industry currently relies on experience and trial and error to design and optimise manufacturing methods. Manufacturing trials however are very costly, and due to the complexity of modern composite systems and the large number of process parameters involved, understanding their impact on product quality presents a significant challenge. Hence, process models that can predict deformation and the final geometry of the part are becoming increasingly desirable.

Fibre path defects commonly form during consolidation prior to curing, because of the compliance of the uncured prepreg plies. Belnoue et al. presented a phenomenological analytical model which considers the transition from squeezing to bleeding flow, which was experimentally observed by Hubert and Poursatrip. The model was validated using experimental data and was implemented as a hyper-viscoelastic material model in a commercial finite element package, via a user material subroutine. It was later successfully used to investigate wrinkle formation mechanisms in lab-scale, industrially relevant geometries. However, the ply-by-ply approach utilised was computationally expensive, making it unlikely to be effective in the design phase of real-size components in industry. To tackle this issue, a kinematically enriched constitutive modelling approach, inspired by the work of Nguyen et al., was developed to predict the mechanical response of the prepreg ply stacks. This method was also implemented in a commercial finite element package via a user material subroutine. It was successfully used to predict wrinkles on the same geometries as the high-fidelity approach, which served to validate the new modelling framework. It was shown to be computationally efficient enough to be used as a design tool, allowing the evaluation of a wide range of geometrical configurations and process parameters. However, due to the "homogenisation" of the laminate which is employed by this method, detailed information on individual ply deformation and interaction was not captured.

In the present contribution, the effort to create a post-processing tool for the kinematically enhanced constitutive modelling approach in order to calculate and visualise the deformation of the individual plies is described. In the "homogenised" laminate simulation, the homogenised strains and strain rates are decomposed in the individual layers at every time increment. Therefore, it is possible for the strains of each layer to be extracted from the simulation and be mapped back onto a ply-by-ply geometry, making it possible for the deformation of the individual plies to be visualised in a much more computationally efficient way than the original high fidelity approach.

A study of a highly tapered thick composite laminate using the updated process is described. Initially, the consolidation of a baseline laminate was simulated using the "homogenised" modelling framework. During the simulation, the individual ply strains were extracted and used to calculate the ply displacements, which were then mapped back onto the initial ply-by-ply geometry. The new approach was then used to numerically study the effect of ply length and thickness variability on the quality of the finished part. The variability study results are discussed.

Multiscale Stochastic Analysis of Short Fiber Reinforced Composites Fabricated by the Injection Molding Considering Random Variation in Fiber Orientation Distribution

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Key Words: *Short fiber reinforced composite material, Fiber orientation distribution, X-ray computed tomography, Injection molding, Multiscale stochastic stress analysis*

Composite materials have superior specific strength and stiffness to homogeneous materials, but the material properties of composite materials are more complicated than those of single materials. For example, in fiber reinforced composites, variations in the component material properties and shape of microstructure have a complex effect on the apparent average properties of the composite. Therefore, the analysis of these effects has been reported in recent years [1].

The injection molding is one of the methods for forming process of short fiber reinforced composites. In the case injection molding using short fiber reinforced resin, fiber orientation and fiber shape can have a significant influence on the mechanical properties of molded products. Therefore, analysis that considering the properties of fibers in molded products have been reported [2]. In the previous reports, fiber orientation was assumed to be uniformly distributed random variable. However, in fact, the velocity distribution of the resin during filling and the cavity pressure are considered to affect the fiber orientation. In recent years, necessity of considering the fiber orientation in molded products has been recognized. However, in injection molding process, the properties were not identical for each molded product even in case of manufacturing same conditions, and inaccuracy was observed in the properties. Therefore, a stochastic analysis that takes these factors into account will be needed.

In this paper, injection molded specimens reinforced by short fibers were subjected to x-ray computed tomography (CT) to extract the three-dimensional fiber orientation distribution and fiber length, and a stochastic analysis was performed with a detailed numerical model reflecting the fiber characteristics of the short fiber reinforced composites. Referring to the measured fiber orientation angle and fiber length as stochastic parameters, stochastic homogenization and stochastic microscopic stress analysis are attempted using Monte Carlo (MC) simulation and multiscale analysis. Influences of random fiber orientation and fiber length variation on probabilistic characteristics of apparent mechanical properties and microscopic stresses of short fiber reinforced composites fabricated by injection molding are investigated.

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Relation between Cutting Resistance and Crack Progress

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Key Words: *Cutting Resistance, Fracture Mechanics, Energy Release Rate, Trace Control, Robotic Arm*

When materials are cut with a knife, cutting resistance is a combination of (1) the reaction force (compressive) and (2) the frictional force between the knife edge and materials. When cutting resin material, the frictional force is dominant, and this mechanism is effectively used for cutting resin material for final shaping, under supersonic motion of Piezo electric material.

Meanwhile, in the field of fracture mechanics, crack progress possibility is evaluated by the stressintensity factor which is calculated from energy release rate around crack tip. In this context, a model of wedge shape rigid body and V-shaped groove is prepared for a reciprocating motion, in which the tangential friction force and the energy release rate are calculated. As a result of this calculation, the maximum energy release rate is obtained at the fore end of wedge motion.

In addition, thick plates with rectangular shape and arc shape are prepared, which are under the moving concentrated force and the gravity force. In this case, the element death function is used effectively for modelling the material vanish, and free fall of material due to the gravity force.

As an experimental validation, the experimental setup is prepared which is composed of robotic arm, and a supersonic cutter at the tip of the arm. Because this cutter penetrates the resin plate reciprocally at a high speed, the cutting resistance reduces significantly. For example, when a CFRP plate is continuously cut, the cutting resistance is reduced by 0.8(%), 1.5(%) and 3.8(%) for CFRP plate with the thickness of 0.5(mm), 1.0(mm) and 2.0(mm) respectively.

On the other hand, when the high speed supersonic cutter is activated, the temperature of the CFRP plates with the thickness of 0.5(mm), 1.0(mm) and 2.0(mm) rise up to 47(deg), 56(deg) and 84(deg) respectively. According to the earlier study, the tensile stiffness reduces 20(%) when the temperature of CFRP plate rises higher than 60(degC).

In other words, the high speed motion of the supersonic cutter causes the friction force between the cutter and the material, and at the same time, the temperature rise of the material. Further study is needed to clarify which mechanism is dominant for the reduction of the cutting resistance.

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Development of atomistic simulation approach at diffusive time scale: an extension of cluster activation method to a continuous space

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Key Words: *Computer Simulation, Cluster Activation Method, Diffusive Time Scale, Solidification, Grain Growth, Grain Boundary Energy*

Atomistic behaviours in metals and alloys have been broadly investigated using molecular dynamics (MD) simulation. The applicability of MD simulation, however, is limited to a phenomenon at relatively small time scale because of its large computational burden. Recently, phase-field crystal (PFC) method has attracted lots of attentions because it can simulate atomistic behaviours at diffusive time scale [1]. The PFC method is versatile, and a variety of phenomena have been simulated, such as solidification, phase separation, and dislocation dynamics. However, it is basically a phenomenological approach, and a determination of input parameters in PFC method is not an easy task, which limits the applicability. In this work, a new atomistic simulation model is proposed, which is an extension of cluster activation method (CAM) [2, 3] from discrete to continuous spaces.

The original CAM is a method of statistical mechanics based on discrete lattice and can simulate solid-solid phase transformations, such as phase separation and ordering phenomena, by solving master equations that determine a time evolution of occupation probability of each atomic species at Bravais lattice points [2, 3]. By extending the method to a continuous space, which is called continuous CAM in this work, local atomic displacement, dislocation, grain boundary, and liquid phase can be represented using the occupation probability at each grid point which is finely distributed compared to the Bravais lattice spacing.

In this work, a variety of phenomena in a pure metal, such as solidification, nucleation of solid, and grain coarsening, was simulated using continuous CAM, where Lennard-Jones potential was employed for the simplicity. It was confirmed that a quite similar solidified microstructure with PFC method [4] can be produced by continuous CAM. Furthermore, the dependency of grain boundary energy on orientational mismatch between neighbouring grains fits well with the Read-Shockley equation for small misfit orientations. It is noteworthy that the continuous CAM employs interatomic interaction energies as main input parameters, which is in contrast with the fact that the PFC method needs phenomenological input parameters.

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Effects of Grain Sizes on Mechanical Behaviors of Nanoglasses

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Key Words: *Nanoglass, Kinetic Monte Carlo Mesoscale Model, Eigenstrain, Grain size*

The most intrinsic way to improve the ductility of amorphous alloy is to impede the occurrences of shear bands. A new conceptual amorphous alloy, nanoglass (NG), which is composed of grains with glassy interfaces has gotten numerous attractions [1]. Simulations and experiments have also shown that NGs possess more ability to accommodate plastic deformation rather than metallic glasses (MGs) [2]. To investigate the effects of grain sizes on mechanical behaviors of NGs, we develop a kinetic Monte Carlo mesoscale model. In the proposed model, eigenstrains with Gaussian distribution are utilized to characterize the plastic strains of amorphous alloy. Moreover, a new softening mechanism which increases the standard deviations of eigenstrains in local shear transformation zones (STZ) according to the von-Mises plastic strain is proposed to decrease the activation barriers of STZs. Numerical results reveal that the ductilities of NGs are dominated by grain sizes. The flow stress in the stress-strain curve drops from severely to gradually by decreasing the grain size. In addition, the strain distribution of NGs transforms from a single shear band to homogenous deformation when the grain sizes decreased. Parametric study is also performed to investigate the effects of STZ modes on the mechanical behaviours of NGs.

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The Optimization of Band Gap in Phononic Crystal and Acoustic Rectification Design using Genetic Algorithm

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Key Words: *Phononic Crystal Plate, Genetic Algorithm, PZT Transducer*

The wave rectification devices can be applied in the areas of noise/vibration isolation, speech signal processing and medical ultrasonic imaging. Among them, a lot of research effort has been directed to the design and implementation of acoustic/elastic wave diodes[1,2]. In this study, we attempted to design a elastic wave diode on phononic crystal (PnC) plate with the properties of partial bandgap, which means wave would be blocked along some, but not all, directions. The genetic algorithm was adopted to carry out the topology optimization for the periodic hole structure on PnC plate to achieve the maximized partial band gap between two prescribed consecutive dispersive branches. COMSOL Multiphysics was adopted to analyze the band structure and the corresponding modes for all the unit cells. The dispersive waves can be classified as symmetric, antisymmetric Lamb wave and non-Lamb waves by the modal judgment. It was assumed the unit cell was arranged in square lattice. The genetic algorithm was employed to design the unit cell in order to achieve the maximization of full or partial band gaps under the constraint of filling ratio. The full wave calculation was used to calculate the wave transmission of the design structure on PnC plate as numerical verification. Experimental measurements were also carried out using ceramic piezoelectric transducer on the optimized periodic stucutre of the plate.

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Ultra-large atomistic simulations and decentralized post-processing analysis for NiTi shape memory alloys under indentation process

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Key Words: *Visualization, Graph Neural Networks, Shape Memory Alloys, Microstructures, Crystal Variant, Ultra-large atomistic simulation, Taiwania3*

Shape Memory Alloys (SMAs) have outstanding mechanical and thermal coupling properties, and also exhibit unique properties when subjected to external environmental stimuli. These properties are dominated by microstructural evolution in nanoscale to mesoscale. This indicates that size effect is an issue in the corresponding atomistic simulations. In the current work, the service of supercomputer, Taiwania3, provided in NCHC in Taiwan, is used to enable ultra-large molecular dynamics (MD) simulation for the indentation process in NiTi SMAs. The model size is up to 250 nm * 250 nm * 210 nm, with 800 million atoms with the indentation depth of 9 nm.

While common post-processing methods, such as CNA[1] and PTM[2], can only distinguish the difference between austenite and martensite phases[3], a graph neural network based post-processing tool, MVIM-G, is used here to illustrate the martensite variants based on the phase transformation matrices. Thus, the detailed martensite microstructure, including the orthorhombic, monoclinic, and R phases in SMAs can be revealed in our model. In addition, for such the huge computational results, a decentralized computational approach is needed to investigate the microstructure evolutions during the indentation. The results are divided into thousands of independent pieces based on their spatial relationship, and are visualized by parallel rendering. The current work eliminates boundary and size effects in the MD results and is expected to be beneficial to the field of atomistic study and simulation.

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Mechanical Properties of Filled Carbon Nanotubes with Greenhouse Gas Mixtures

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Key Words: *gas mixture, interface, mechanical properties, confinement*

The increasing demand for higher CO_2 capture rates is driving novel and sustainable carbon removal processes. Membrane separation is one of the leading gas capture technologies. Carbon nanotubes (CNTs) [1], due to their unique properties, have been considered promising materials for developing the next generation of membranes [2,3]. A fundamental understanding of these systems' mechanical properties is essential for such applications. In this context, molecular dynamics (MD) simulations were carried out to investigate the mechanical properties of single-walled carbon nanotubes (SWCNTs) filled with CH_4/CO_2 gas mixture under tensile and compressive strain. Initially, armchair (*ar*) and zigzag (*zz*) SWCNTs were loaded with CO_2 and CH_4 using Grand Canonical Monte Carlo simulations. MD simulations were conducted at temperature and pressure of 313.15K and 200 atm, respectively. The nanotube's diameters range from approximately 8 to 19 Å, and the number of molecules varies according to the nanotube's size. For instance, the smaller *ar* nanotube has a 50:50 composition (CO_2:CH_4) and 0,0465 molecules/Å^3, while the largest has 72:28 composition and 0,0210 molecules/Å^3. In general, SWCNTs show a higher selectivity towards CO_2 than CH_4. Under tension, filled SWCNTs present a similar mechanical response to empty ones, regardless of the gas composition, chirality, and diameter. We also observed that the fillers do not affect the nanotubes' fracture and buckling patterns compared to the empty nanotubes. Overall, the filled SWCNTs' mechanical behavior is similar to the empty ones when under tension, showing a minor effect of the gas composition on their performance. Our results confirm carbon nanotubes as promising nanostructures for applications involving gas separation.

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Nanoscale Mechanical Energy Storage based on Spiral Spring

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Key Words: *Mechanical Energy Storage, Diamane, Energy Density, Atomistic Simulation*

Electro-chemical batteries such as lithium-ion batteries (LIBs) that have a high energy and power density (from 150 to 300 Wh/kg) and long life-span are the most popular portable power supplier in our modern society[1-2]. Whereas, huge battery consumption not only causes excessive usage of minerals or strategic materials, but also lead to a large amount of end-of-life battery packs that threaten the environment and human health. At small scale, researchers have demonstrated that micro-/nanoscale biomedical robots are capable of carrying out a wide range of tasks including surgery, gene therapy, drug delivery, diagnosis, and other tasks that are hardly achievable traditionally. The practical engineering deployment of high-end electromechanical systems/devices, especially in harsh or biological environments (like outer space and deep-sea exploration, and biomedical applications), relies heavily on the development of a compact, stable, safe, sustainable, and high-energy density storage/power supply system.

This work proposed a spiral-based nanoscale mechanical energy storage scheme utilizing the newly synthesized two-dimensional (2D) diamane. Such spiral structure or 1D van der Waals structures have already been successfully fabricated based on different 2D nanostructures[3-4]. Atomistic simulations show that the diamane spiral can achieve a high theoretical gravimetric energy density of about 564 Wh/kg, about 14500 times of steel spring. Fundamental principles that dominate the limit of energy storage in the contact spiral and tracked spiral are discussed in detail with the corporation of theoretical models, respectively. The obtained insights suggest that the 2D vdW solids could be promising candidates to construct spiral structures with a high gravimetric energy density.

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Abstract details:

Tensile Performance of Polymer Nanocomposite with Randomly Dispersed Carbon Nanothread

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Keywords: Polymer Nanocomposite, Carbon nanothread, Random dispersion, Functionalized fillers, Mechanical Property, Molecular Dynamics Simulation

Summary of presentation

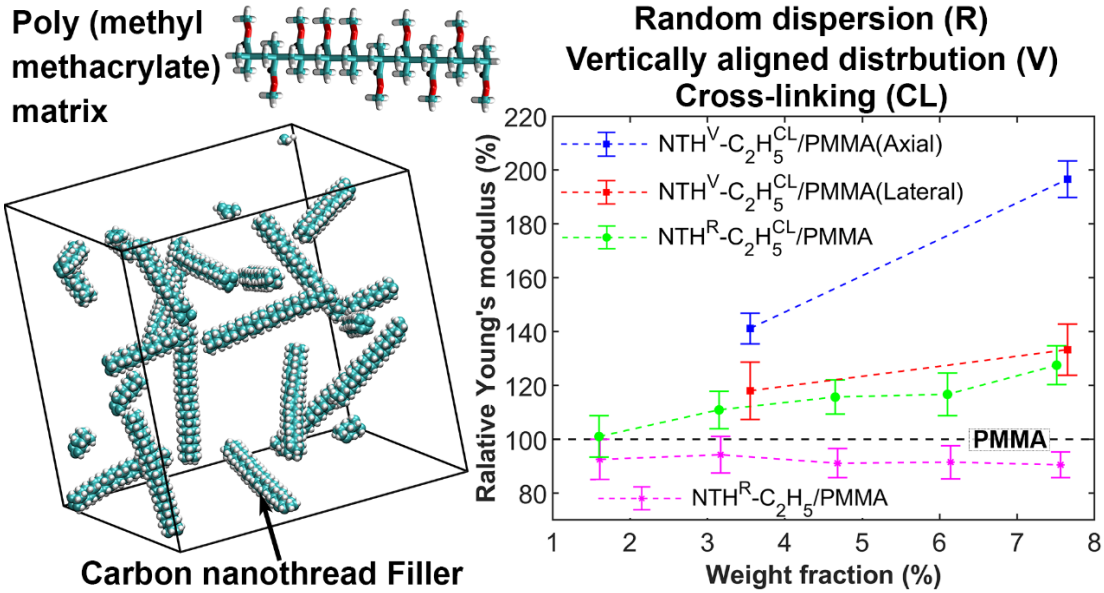
This work investigates the role of the random dispersed carbon nanothread (NTH) to reinforce poly(methyl methacrylate) (PMMA) nanocomposite. It is found the 1D fillers cause deterioration in the tensile properties due to the weak intermolecular force and enlarged continuous interphases within the PMMA matrix. The PMMA sample with 6.0% NTH is about 2.38±0.18 GPa (~19.1% smaller than PMMA). Further investigations reveal introducing functional groups (such as 13% –COOH functionalized NTH) can turn the negative impacts into positive enhancements. Furthermore, Young's modulus received up to 27.5% increment than pure PMMA for

the presence of covalent bonds between NTHs and PMMA chains due to the effective load-transfer. It is noteworthy that the enhancement is significantly influenced by the NTHs' length, weight fraction, functionalized and cross-linking percentage. In addition, the ideal samples with vertically aligned NTH fillers are further investigated and compared, the cross-linking can further enhance axial and lateral Young's modulus (up to 96.6% and 33.2% higher than PMMA). Specially, a high cross-linking percentage causes additional voids due to the inconsistent movement between cross-linked and non-cross-linked PMMA chains. These results signify the importance of dispersion and interfacial modification toward better mechanical performance, which should shed light on the design and fabrication of high-performance polymer nanocomposites.

Contribution

Low-dimensional nanostructures have been widely used as reinforcements for polymer nanocomposites. However, majority of studies have considered the samples containing a single or perfectly aligned nanofillers, which is usually not the case for the as-synthesized samples. Through molecular dynamics simulation, this work systematically assessed the tensile performance of poly(methyl methacrylate) (PMMA) nanocomposite with randomly dispersed carbon nanothread (NTH) - a new one-dimensional ultrathin nanofiller. It is found that NTH causes deterioration on the tensile properties due to the introduction of continuous lower density interphases surrounding the filler, while such negative impacts can be turned into positive enhancements by functionalization. In particular, the cross-linking at the NTH/PMMA interface is able to effectively promote the enhancement effect from the nanofiller. Our results show that the samples with random but vertically aligned NTHs outperform their counterpart with randomly dispersed NTHs. Overall, it is shown that the enhancement effect is significantly influenced by the NTHs dispersion, length, weight fraction, functionalization and cross-linking. This study provides a comprehensive understanding of the influence on the tensile performance of polymer nanocomposites from the dispersion of nanofillers, which should benefit on the fabrication and

application of high-performance polymer nanocomposites.



Vacancy Diffusion in Nickel Alloys under High Pressure through Atomistic Simulations

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Key Words: *Nickel Alloys, Vacancy Diffusion, High-pressure, Collective Variable-driven Hyperdynamics*

To achieve high propulsion ratio requirements for aero engines, the stress on the engine blades is getting higher and higher [1,2]. Due to the outstanding creep performance, nickel-based single crystal superalloys become a key material for aeroengine blades. The creep phenomenon is a long-time deformation process that involves with dislocation movement, grain sliding, and directional diffusion. It is critical to study the vacancy diffusion in nickel-based single crystal superalloys, especially under high-pressure as induced by the high centrifugal force in aero engine. Due to the limitation of time scale, traditional molecular dynamics (MD) is unable to capture the infrequent vacancy diffusion event [3]. In this study, collective variable-driven hyperdynamics (CVHD) is used to accelerate the vacancy diffusion event in the Ni-Al-Re superalloys with varying pressure. As expected,, the diffusion rate of vacancies in the nickel-based single crystal superalloys increases when the pressure increases. This work provides atomistic insights for the diffusion phenomenon in Ni alloys, which could benefit the design of next-generation high-performance alloys.

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Bandgap property of a metaplate with multiple resonators

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Key Words: *metaplate, bandgap, flexural wave motion, membrane-mass system*

Acoustic metamaterials possessing unusual properties have been viewed as good candidates for the manipulation of elastic/acoustic waves. Liu et al. [1] first presented the advantage of the local resonant mechanism which broke the phononic crystals' limitation. Since then, this novel concept has been widely applied in various kinds of engineering structures. There are many different types of forms in locally resonant units, such as a spring-mass system [2,3], a soft rubber cylinder in epoxy host [4], a spiral structure [5], and a beam-like structure [6]. The decorated membrane resonators also has shown their good performance in wave blocking at low frequencies [7]. By adjusting the geometric or physical properties of the resonator, the desired bandgap range can be achieved. In this study, a metamaterial plate consisting of a perforated plate equipped with multiple membrane-mass systems is proposed. A theoretical model based on extended plane wave expansion method is developed to predict bandgap location and width for the present structure. Finite element simulations and experiment measurements are carried out to verify the analytical results. Parameter studies are conducted to reveal the effect of parameters on bandgap property. The use of the double-layered structure can increase the bandwidth of the attenuation zone.

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Designing Composite Materials via Genetic Algorithm and Conditional Variational Autoencoder

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Key Words: *Composite Material, Machine Learning, Genetic Algorithm, Finite Element Method, Tensile Test, 3D Printing*

Designing composite materials with tailored stiffness and toughness is challenging due to the astronomical number of possible material and geometry combinations. Although various studies have applied machine techniques and optimization methods to tackle this problem, we still lack a complete understanding of material effects at different positions and a systematic experimental procedure to validate the results. Here we study a 2D binary composite system with an edge crack and grid-like structure using Genetic Algorithm (GA) [1] and Conditional Variational Autoencoder (CVAE) [2], which can design composite with desired stiffness and toughness. We use finite element simulations to generate a machine learning dataset and perform tensile tests on 3D-printed specimens to validate our results. We show that adding soft material behind the crack tip, instead of ahead of the tip, tremendously increases the overall toughness of the composite. We also show that while GA generates composite designs with slightly better accuracy, CVAE takes considerably less time to generate designs. Our findings may provide insights on the effect of adding soft material at different locations of a composite system and may also provide guidelines on conducting experiments to validate the results.

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Modelling Mechanical Properties of Nanocomposites with Aligned graphene Platelet

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Key Words: *Nanocomposites, Mechanical Property, Graphene Platelet, Modelling*

This study aims to characterize the mechanical properties of nanocomposites with aligned graphene platelets. Both analytical model and experiments were conducted and the results were compared with each other. For the modelling, the mechanical properties of nanocomposites were characterized using Mori-Tanaka micromechanical model in which the graphene platelets were assumed to be disk-like plates aligned in one certain direction. The distribution of the aspect ratio of the platelets and the orientation of the graphene plates were considered in the micromechanical model. On the other hand, the nanocomposites were fabricated by compounding the epoxy resin and graphene platelets using mechanical mixer together followed by sonication. The mixture of graphene platelets and epoxy was subjected to electrical field in order align the graphene platelets. Coupon specimens with the aligned graphene were tested under tensile loading. The Young's moduli of the nanocomposites with different degree loadings of graphene platelets were measured and the results were compared to the model predictions. Results indicated that the micromechanical model can characterize the mechanical properties of the nanocomposites with the aligned graphene platelets.

Seed-pod-inspired Shape Transformation via 4D Printing

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Key Words: *Seed pods, shape transformation, 4D printing*

Plant tissue can perform complex motion via shape transformation to achieve various purposes—this effect origins from the interaction between multi-scale structures and mechanical properties in plant materials [1]. For example, pine cones absorb water to fold scales to prevent seeds from damp [2].

Bauhinia x *blakeana*, or the Hong Kong Orchid Tree, is a natural hybrid of great horticultural value cultivated in gardens, streets, and parks. Its seed pods open between April and August and have two distinctive chirality-creating mechanisms, referred to as "inversion" and "eversion" here—the initially flat pod valve is turned into a helix but with different chirality. Inversion tends to occur around April, whereas eversion tends to occur later in August. Previous studies have discussed the shape transformation of many kinds of seed pods and utilized simulation and synthesis gel models to verify the transformation mechanism [1, 3]. However, it is still unclear how these two different helical morphologies may be created by changing the layered structure and composition. In this paper, we create a multi-layered seed pod model by 4D printing to reproduce inversion and eversion morphology. We then speculate how the seed pods transform. 4D printing, a combination of 3D printing and active materials, is convenient and controls the deformed shape through parameterization. By contrast, the conventional gel model requires a molding process and cannot be easily parameterized. Furthermore, we verify the feasibility of the 4D printing model by simulation, and the results are consistent. In the future, we will investigate the microstructure of the layered cells in the seed pods and measure the mechanical properties of the plant materials, which will be used to fine-tune our 4D printing model to mimic the actual situation of the *Bauhinia blakeana* seed pods.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Molecular Dynamics Simulation on Carbon Nanocoil with Flat Ribbon Cable Shape

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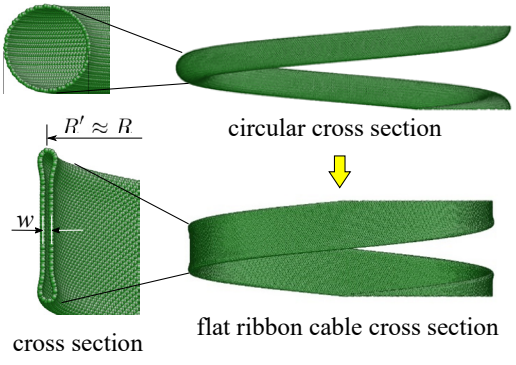
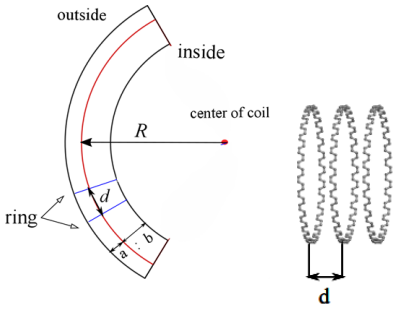
Key Words: Carbon Nano-Coil, Molecular Dynamics Simulation, AIREBO Potential

Contrary to straight carbon nanotubes, there is no theoretical model for carbon nanocoils (CNC) due to the difference between internal and external diameter of the coil. Some researchers performed molecular dynamics simulations on CNCs[1, 2]; however, simulated CNCs usually show kink and facet shape due to buckling of internal circle. Here we obtained a CNC with flat ribbon cable shape (referred as FRCNC) from initial circular tube made of unit rings of zigzag or armchair carbon nanotube (CNT), by molecular dynamics simulation with AIREBO potential. FRCNC has no defect or all carbon atoms show six-membered ring. The formation of FRCNC depends on the relationships between the unit ring radius (or tube radius), unit ring structure (zigzag or armchair), coil radius and the initial location radius R where the ring distance d is set to that of natural C-C bond length (right schematic). On the other hand, formed FRCNC always shows R' almost identical to the location radius R, and the flat ribbon width w is almost constant, $w \approx 0.34$ nm. This value is the equilibrium distance between graphene sheet in AIREBO potential. Thus the obtained FRCNC maybe a potential dependent phenomena; however, we discuss the formation mechanism and mechanical properties of the FRCNCs as a new type of carbon material.



(a) snapshots of initial and final configuration



(b) location of natural C-C distance in initial array of CNT ring unit

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Molecular Dynamics Simulation On Mechanical Properties and Deformation Mechanism of Graphene/Aluminum Composites

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Key Words: *Graphene/Aluminium composites, Mechanical properties, Deformation mechanism, Molecular dynamics simulation*

In this paper, the mechanical properties of the Graphene/Aluminium (Gr/Al) composites under uniaxial tensile and compression were investigated using molecular dynamics (MD) simulation method. Six different simulation models are used to investigate that graphene significantly improves the stiffness and strength of Gr/Al composites. Moreover, the research results shows that the existence of graphene layer can effectively prevent the propagation of dislocations at the interface, so the mechanical properties of the composites are improved. The dislocation movement of Al matrix during compression was further investigated. It was found that stair-rod dislocation and hirth dislocation occurred in Al matrix, which was helpful to improve the mechanical properties of the composites. In addition, the average curvature of compressed graphene surface is measured, and the deformation characteristics of composite graphene are considered by geometric method. The deformation mechanism of composites is studied by comparing the effects of deformation behavior, compressive stress, potential energy and dislocation.

Optimal Shape Design of Graphene Sheets by Introducing Lattice Defects

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Key Words: *Frequency, Graphene Sheets, Lattice Defects, Optimal shape design, Stiffness*

Since they were produced in 2004 [1], graphene sheets (GSs) have been attracted plenty of attention among scholars because of their superior material properties. In especial, GSs have been supposed to be the base materials adopted in nanoelectromechanical systems (NEMS) [2].

In this study, we foucs on two basic mechanical properties, stiffness and fundamental frequency, of GSs and propose a consistent optimal shape design methodology of GSs by introducing lattice defects. This methodology consists of the molecular mechanics (MM) method, the free-form optimization method, the Phase-Field-Crystal (PFC) method, Voronoi tessellation, and molecular dynamics (MD) simulation. Details are shown as following.

At first, based on the MM method, C–C bonds of GSs are simulated as equivalent continuum beams by a combination of molecular and continuum mechanics [3], so the atomic structures of perfect 2-dimensional GSs, i.e., the initial shape of GSs, can be treated as frame structures. Then, we adopt the free-form optimization method for frames [4] to determine the optimal shapes of GSs in stiffness maximization problem and fundamental frequency maximization problem. However, the obtained optimal shapes and GSs do not satisfy the stationary-action principle due to the complicated interatomic force among carbon atoms. Hence, to obtain the stable atomic structures of the determined optimal shapes of GSs, we introduce lattice defects in the optimal shapes of GSs using a combination of PFC method, Voronoi tessellation, and MD simulation [5].

The optimal results [6,7] show that the stiffnesses or the fundamental frequencies of given GSs can be significantly enhanced using this proposed methodology, which is helpful for designing GSs as base materials in NEMS.

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Vibration Characterization of Multi-Walled Carbon Nanotubes with Different Lengths

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Key Words: *MWCNT, vibration, natural frequency, interlayer distance*

Since 1991 after the discovery of carbon nanotube (CNT), CNT plays an important role in the field of nanotechnology because of their unique structural, mechanical properties and electrical properties [1][2]. The density of CNT is very low which is about half of aluminium, and the strength of CNT is about 20 times stronger than steel, making them an excellent material with high natural frequencies. In this study, we aim to design a model which can considered to be used as a nanoscale sensor by using Multi-Walled Carbon Nanotubes (MWCNT) which has higher frequency than the Single-Walled (SW) CNT. The vibration analysis of MWCNT is performed using the molecular dynamics (MD) method. We design different kinds of MWCNT including SWCNT, Double-Walled (DW) CNT, Triple-Walled (TW) CNT and Quadruple-Walled (QW) CNT with different lengths, similar to the shape of a probe. The diameter of the innermost layer CNT in the analytical model is 3.892Å. The interlayer distance of the MWCNT is set to be the same value which is Δr=3.114Å due to the van der Waals force between the adjoined layers. The results show that with the increasing of layers of MWCNT, the natural frequency becomes higher. Then, we use QWCNT as our model for vibration analysis by changing the radius of the innermost layer. The interlayer distance of the QWCNT is set to be around Δr=3.114Å, and the height of each layer is fixed in this simulation. The results show that the natural frequencies become higher, when the radius of the innermost layer increases. In next simulation, the radius of the innermost layer of the model QWCNT is set to be 1.946Å, and interlayer distance is set to be around Δr=3.114Å. The results show that the natural frequencies become higher, when the length of the QWCNT decreases. From these results, MWCNT has high natural frequency, and it is highly likely to be utilized as a nanoscale sensor.

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Application of Isolated Element Method to Fracture Mechanics Analysis

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Key Words: *Isolated Element Method, Fracture Mechanics Analysis, Stress Intensity Factor*

This paper presents an application of the isolated element method (IEM) to fracture mechanics analysis. In the IEM, the body of interest is described as a collection of isolated elements [1]. The displacement functions are defined independently for each isolated element. The principle of minimum potential energy that is expanded to satisfy the continuity of the displacement at the interface between neighbouring isolated elements is applied. Using these remarkable properties of the IEM over the conventional finite element method (FEM), the IEM is applied to fracture mechanics problems. In the IEM, the local refinement of isolated elements near the crack tip can be achieved without smooth connection of neighbouring isolated elements. In addition, higher order displacement function and the displacement function for crack tip can be locally used for isolated elements near the crack tip. These special techniques can enable us analysing the fracture mechanics problems without extensive efforts to generate finite element mesh with a particular design near the crack tip and with a sufficient numerical accuracy.

As a demonstration of the application of the IEM to fracture mechanics problems, a plate with a crack under tension loading is analysed. The problem has a simple geometry and boundary conditions, and thus, symmetric (displacement) boundary condition can be applied. In the symmetric boundary condition, the displacement in the loading axis direction is fixed at the ligament part of the crack. However, the displacement in the IEM solution at the ligament part cannot be perfectly fixed. The stress intensity factor calculated using the displacement extrapolation method also has a subsequent numerical error. To improve the numerical accuracy of the IEM in the fracture mechanics analysis, the displacement function of the isolated elements at the ligament part is rearranged to satisfy the displacement boundary condition. The centre of the displacement function is shifted to the ligament part, and some terms in the displacement function is removed to completely satisfy the displacement boundary condition. The numerical results using the special displacement function at the ligament part shows a perfect satisfaction of the displacement boundary condition. Using the numerical solution of the displacement near the crack tip, the stress intensity factor is calculated. The numerical accuracy of the stress intensity factor can be drastically improved compared to the IEM solution without the special displacement function. Furthermore, the crack tip displacement solution is embedded into the displacement function for isolated elements near the crack tip. We found that the application of the crack tip displacement function can also improve the numerical accuracy of the stress intensity factor calculation.

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Application of Machine Learning for Accurate and Efficient Simulation of Radiation Damage Formation in Metals for Nuclear Reactors

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Key Words: *Radiation damage, Molecular Dynamics, Binary Collision Approximation, Machine learning*

For the safe operation of nuclear reactors, it is important to understand and control the effects of radiation damage on the mechanical properties of nuclear materials. Radiation damage consists of various processes occurring on different time scales, such as the radiation damage formation in ns~ps, the recovery of radiation defects just after the formation in ps~ns, and the long-term evolution of defect complexes in hour~year. For the radiation damage formation process, two computational methods have been widely used. One is the binary collision approximation (BCA) [1] and the other is the molecular dynamics (MD). BCA has the advantage of high computational efficiency because it approximates many-body atomic collisions to two-body atomic collisions, but it cannot give accurate defect structures due to its approximation. On the other hand, MD can simulate many-body collisions as they are, and thus can give an accurate defect microstructure if an accurate potential model is prepared. Therefore, in order to achieve accurate and effective computer simulation of radiation defect formation, it is important to seamlessly couple BCA and MD and to prepare an accurate potential model for MD. In this paper, we present our recent attempt to solve these two problems by applying machine learning (ML).

For seamless coupling of BCA and MD, we constructed two machines based on the MD collision simulation results up to several tens of keV. Specifically, one machine generates a pseudo-random defect structure satisfying statistics such as defect number distribution and defect position distribution, referring to the MD simulation results. The other machine is trained to classify the MD-generated defect structure and the random defect structure, and determines whether the generated quasi-random defect structure by the first machine is reasonable or not. By using the BCA code until the damage energy becomes several tens of keV, and then switching to the machines, we can generate defect structures similar to MD at a speed comparable to BCA.

To create a highly accurate MD potential model, we constructed a moment tensor potential [2], a kind of ML potential model, by referring to the results of first-principles calculations for various defect structures and material properties. The constructed ML potential model agrees well with the first-principles calculations and shows much better performance than the conventional potential model. It was confirmed that the generated ML potential can be used stably in collision simulations. In this presentation, we will discuss an effective way to generate ML potentials for radiation damage simulations.

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Designing an open structure based on atomic-level structural configuration for higher elastic modulus

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Key Words: *Open structure, finite element method, elastic modulus*

In this study, the authors create various open structures that reflect an atomic-level structure database. And we design open structures with higher Young's modulus, shear modulus and bulk modulus. In a modeling process for the open structure, the atomic positions were imported from the Materials Project, an open access materials database. Then we modeled open structures by considering the atomic positions as vertices and connecting them with circular 1D beams. As a result, open structures were modeled with various atomic arrangements belonging to different space groups. In a test process, the mechanical properties were calculated by compression along the x-, y- and z-axis using the FEM tool. Authors introduce open structures with the higher Young's modulus, shear modulus and bulk modulus. We discuss what geometric factors strongly affect the moduli of elasticity in open structures.

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Durability and Aging of Composites under Environmental Deterioration and Fatigue

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Key Words: *Composites, Deterioration, Ultraviolet Radiation, Moisture, Heat, Homogenization, Fatigue, Damage, Flexure*

Glass fiber-reinforced polymer composites (GFRPs) are made by combining polymer with reinforcement glass fiber yarns to produce lightweight yet strong materials. This study is to build a Multiphysics and Multiscale model to predict the synergistic effect of environmental exposure to fatigue-damage of the composite.
Based on the authors' previous UV/moisture exposure experiment-computational study, this extended study couples environmental deterioration induced material weakening to continuum fatigue-damage model. The extended research developed a fatigue-damage model at the structural length scale, using diffusion coefficient tensor and stiffness tensor homogenized from a plain-woven RVE at mesoscale length scale. The experimental validated computational model shows that environmental exposure causes material degradation, which leads to a mild change of damage variable field and considerable change of fatigue parameter after 1000 hours of accelerated cyclical UV/moisture exposure. The synthetic effects of these two changes reduce structural stability. The most significant effect is observed by measuring bending moments after the tension-tension fatigue test. After 100,000 cycles, the bending moment of cyclic UV/moisture degraded samples decreased up to 40 percent compared to undegraded samples. This model can be incorporated into many commercial finite element codes for a sustainability study of composite structures/systems. In future work, the models developed in this study will be combined with life cycle assessment (LCA) tools to better support sustainability focused design of new material, thus reducing costs and environmental impacts of the built environment.

Effects of powder trajectory for Y_2O_3-A_2O_3 interface formation during plasma spray coating: A multiscale analysis

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Key Words: *Multiscale mechanics, Direct simulation Monte Carlo, Molecular dynamics, Plasma spray coating, Yttria thin film*

Yttria is one of the protective materials due to its excellent mechanical and thermal stability. In addition, the tunable bandgap and high dielectric constant make yttria a promising material for optoelectronic devices [1]. This versatile yttria thin film has great advantages in that it can be applied to complex shapes through plasma spray coating [2]. Nevertheless, the plasma spray coating has been performed relying on empirical indicators from numerous experiments. The absence of a theoretical understanding of these plasma spray coatings motivates our works. In this study, we present a multiscale analysis method to explain the origin of interface formation by plasma spray coating.

Our multiscale framework consists of the direct simulation Monte-Carlo (DSMC) method and molecular dynamics (MD). The solution of the Boltzmann transport equation to obtain the trajectory and spatial distribution of powder is approximate through the DSMC methods. Meanwhile, the formation of the interface according to the particle incidence is analyzed through MD simulations.

To evaluate the effect of powder feed and spray distance on the film formation, spatial particle distribution was extracted. The spray cone angle was proportional to the number of powder particles. This tendency is due to the high probability of particle collision in space. Meanwhile, the large cone angle is a major factor in determining the incident trajectory of the particles constructing the interface. We investigate the formation of the Y-O-Al network structure with the incident trajectory of the particles using molecular dynamics simulations. The interface formed by the particles at a gentle incidence angle to the surface had poor adhesion strength as well as a significantly lower density of the Y-O-Al network. These results provide a crucial foundation for analyzing the interface under plasma spray coating.

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Fatigue Crack Growth Simulation of Multiple Surface Cracks Using Discrete Dislocation Dynamics Method

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Key Words: *Discrete Dislocation Dynamics, Fatigue Crack Growth, Multiple Surface Crack, Superposition Principle*

This paper presents an application of the discrete dislocation dynamics (DDD) method to fatigue crack growth simulations of multiple surface cracks. Sheng et al., have developed a DDD based fracture mechanics analysis technique for surface cracks [1]. The boundary conditions of the finite elastic body with cracks can be satisfied by the application of the superposition principle. In the application of the superposition principle, the entire dislocation (crack) problem in a finite elastic body is defined as a summation of a dislocation problem in an infinite elastic body and a correction problem. The correction problem is an elastic problem and is solved by the finite element method (FEM). The boundary condition of the correction problem is determined to eliminate the virtual traction calculated in the dislocation problem. In the calculation of the virtual traction in the dislocation problem, the virtual traction becomes singular along the dislocation line at the free surface. Sheng et al., added a virtual dislocation loop outside the finite elastic body to remove the singularity along the dislocation line at the free surface. Finally, they demonstrated that the DDD based fracture mechanics analysis technique can calculate the stress intensity factor with a sufficient numerical accuracy. In the fracture mechanics analysis using the finite element method (FEM), the elements near the crack tip must be very fine to obtain a numerical solution with sufficient numerical accuracy, and re-meshing is necessary to perform the fatigue crack growth simulation. In some cases, the re-meshing could be a bottleneck to perform the fatigue crack growth simulation particularly of multiple cracks including their coalescence. On the other hand, in the DDD for fracture mechanics analysis, the crack is modelled with a collection of pile-up discrete dislocations, and therefore, the crack shape can be easily modelled and updated by changing the shape of the dislocation line. Therefore, it is easy to deal with the complex dislocation shape and interactions in the fatigue crack growth process.

In this paper, the DDD method for surface cracks is applied to the fatigue crack growth problems of multiple surface cracks. The elastic interaction of multiple surface cracks can be naturally considered in the numerical simulation. The crack geometry change due to the fatigue crack growth is calculated by the Paris law. The crack shape updated by the fatigue crack growth can be easily modelled by updating the shape of dislocation line, which describes the crack front shape. The crack coalescence is also dealt with in the fatigue crack growth simulation. The coalescence can be easily performed as the dislocation annihilation process, which is normally used in the DDD simulation of plasticity, particularly for the Frank-Read source simulation. Finally, as the demonstration of the DDD based fatigue crack growth simulation, the coalescence and penetration of multiple surface cracks are presented.

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Influence of dislocations on hydrogen retention in tungsten

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Key Words: *Molecular dynamics, Hydrogen clustering, PKA, Dislocation, Diffusion*

Recently, tungsten(W) as a plasma-facing-material(PFM) in the extreme environment of nuclear fusion has been spotlighted as an important material in related fields due to its excellent physical properties [1]. However, as the harsh condition of nuclear fusion suffers hydrogen bombardment accompanied with intense irradiations, which leads degradation of the material such as formation of defects and hydrogen embrittlement, it is not easy to guarantee PFMs life [2, 3]. Therefore, understanding the mechanisms and influence of the trapping of hydrogen in neutron irradiated W is important. In this study, hydrogen retention models by Molecular dynamics simulations describing the interaction between H and dislocation are presented. The properties of the W and trapping rate of hydrogen are calculated with varying external conditions such as stress and temperature gradient as well as number and type of dislocations.

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Interfacial properties of Liquid crystal polymer and MWCNT nanocomposite at high filler concentrations: A molecular dynamic study

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Key Words: *Molecular dynamics, Polymer nanocomposites, Mechanical properties, Interface*

Fabrication of liquid crystal polymer (LCP) nanocomposites using a multi-walled carbon nanotube (MWCNT) sheet has attract significant interests as it complements the low mechanical properties and offers multi-functionality [1]. In this study, we investigated the interfacial properties between LCP and MWCNT from the mechanical and structural point of view. The neat LCP and LCP/MWCNT microstructures were constructed in all-atom molecular dynamics environment, and load transfer characteristics as well as internal stress distributions were thoroughly evaluated. Key design consideration of this study is the concentration of MWCNT filler in the nanocomposites. Since the LCP/MWCNT is experimentally fabricated by penetrating liquid crystal into a densified MWCNT sheet, the filler generally has a high volume fraction of 25 % or more. Therefore, different MWCNT volume fractions from 25 % to 48 % were prepared.

To evaluate the alignment characteristics of LCP by interaction with filler, an orientaional order was derived in the radial direction of the MWCNT. In the vicinity of the nanotube surface, the both components constituting LCP, mesogen and side chain, showed high directionality. This is because the rigid core of the LCP consisting of three aromatic rings has the maximum contact area when aligned parallel to the nanotube. These aromatic rings are distributed with two different conformations (parallel and T-shaped alignment) depending on the distance with MWCNT and form a layered structure. In other word, MWCNTs significantly enhance the crystallinity of adjacent LCPs.

To evaluate the interfacial load transfer, tensile simulation of LCP/MWCNT nanocomposites was carried out. The results indicate improved elastic stiffness in both axial and transverse directions as the concentration of MWCNT increases. As the volume fraction occupied by MWCNT increases, the region with high crystallinity in the LCP matrix becomes predominant. This not only greatly improved the effective properties of LCP but also enabled strong coupling with MWCNT, resulting in more effective load transfer.

The present study is the first to explore the interface of LCP-MWCNT at non-dilute filler concentrations. Polymer nanocomposites using MWCNT sheets lacked microscopic insight compared to their experimental novelty. Therefore, this study can be utilized as a guide for the robust design of applications.

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Molecular Dynamics study of Bimetallic Core/Shell Nanoparticles for various Structural Properties in Heat-assisted and Pressure-assisted Sintering process

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Key Words: *Multiscale simulation, Microstructure, Multi-particle modelling, Core/shell Nanoparticles, Molecular dynamics, Pressure-assisted Sintering*

Nanoparticle sintering becomes a new choice for high-temperature packaging for microelectronic applications due to the low sintering temperature of nanoparticles when compared with macro-sized ones while having a good property with high stability. Conventionally, silver nanoparticles are deemed to be ideal because of their high stability, electrical and thermal conductivity, yet the actual usage is limited due to their high price. In this respect, a Cu@Ag core/shell nanoparticle has been suggested by substituting a part of the molecule with the cheaper metal. In addition to a reduction of cost, the core/shell nanoparticle has several advantages of reasonable conductivity and resistance to oxidation.
In this study, we investigate Cu@Ag core/shell nanoparticle sintering using molecular dynamics simulation. Firstly, we investigate heat-induced sintering in terms of melting temperature and microstructure evolution. Additionally, we study the pressure-assisted sintering (PAS), which allows further reduction of pores without excessive heat, preventing damage of heat-sensitive substrates e.g., polymer. We also investigated the effect of interfaces to the sintered structure, which are underpinned by comparing mechanical, and lattice properties of structures with different sintering path.

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Plasma etching time prediction model of high aspect ratio pattern using molecular dynamics with data processing

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Key Words: *Molecular dynamics, Etching, High aspect ratio contact, Data processing*

During the semiconductor process, more than 90% of the etching is performed using plasma. Plasma discharged with various etching gases emits ions with energy and angle distribution, radicals with high chemical reaction rate, and electrons with isotropic velocity distribution to the substrate. These particles are transported into the substrate to be etched, and etching occurs as the conditions of ion-assisted surface activation, heterogeneous reaction by radicals, and charge build up by electron and ion [1]. With the recent development of V-NAND, the aspect ratio of the trench structure risen sharply due to the rapid increase in stack thickness. In the early days of V-NAND, it was possible to predict the situation intuitively for structures with a small aspect ratio. However, it becomes difficult to predict the state of the particles reaching the deep bottom for etching as the frequency of wall collisions of particles transported inside the high aspect ratio pattern increases. Therefore, understanding the states of ions, radicals, and electrons after wall collision is essential for etching prediction. Therefore, in this study, the energy dissipation efficiency, energy loss and angle deviation after wall collision are calculated using molecular dynamics with ReaxFF [2]. Based on the calculated results, a regression analysis with a tendency for the input and output values was performed, and the results of calculating the etching time for each depth from the state of each particle predicted after wall collision were reinforced by learning through Bayesian regularization. At this time, the radicals supplied as a pattern together provide the radical concentration at each depth from the diffusion model reflecting the appropriate diffusivity and rate constant from OES data of plasma. Finally, a high aspect ratio etch time prediction model including charging effect was constructed by adding a component that slows down ions by calculating the electric field formed from charge separation due to the difference in velocity distribution between electrons and ions. Through this model, it is expected that the etching time by plasma state can be predicted in the structure of next generation products.

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Quantitative Evaluation of Kink Strengthening in LPSO-type Magnesium Alloy Using Higher-order Gradient Crystal Plasticity

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Key Words: *Kink Strengthening, LPSO-type Magnesium Alloy, Higher-order Gradient Crystal Plasticity, Meshfree Method*

Magnesium alloys with the long period stacking order (LPSO) structure show the superior strength and are expected as the next generation structural material. In the LPSO materials, kink deformation is an important deformation mechanism as well as slip deformation in the crystalline scale and may be the origin of the material strengthening. Therefore, understanding the kink strengthening phenomena is essential. In the LPSO-type magnesium alloy, band-shaped kink is sometimes observed. Kink band causes the strain gradient around the band. The higher-order gradient crystal plasticity is an efficient way to represent the strain gradient effect in the crystalline scale. In this model, an additional governing equation expressing the dislocation density filed is introduced, and both the displacement and dislocation density fields can be solved simultaneously.

In this study, a higher-order gradient crystal plasticity analysis is conducted to evaluate the stress field around kink band to understand the strengthening mechanism due to kink. The finite element method sometimes provides an improper solution in the higher-order gradient crystal plasticity analysis; therefore, the reproducing kernel particle method, which is a kind of meshfree method, is introduced into the higher-order gradient crystal plasticity analysis.

The numerical result shows there are two main origins of kink strengthening, i.e., the geometrical strengthening and defect strengthening. The former one is also known as the geometrical hardening and caused by the rotation of crystal orientation. The latter one is a strengthening by geometrically necessary dislocation density around the kink boundary. Although both mechanisms cannot be negligible in the kink strengthening, the present result suggests that the defect strengthening is more dominant in the strengthening of LPSO-type magnesium alloy.

Reduction of Interstitial Mobility in W by Transition Metal Multicomponent Alloying

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Key Words: *First Principles Calculations, Interstitial Defects, Alloys*

Tungsten (W) is one of the promising base materials for plasma facing components in fusion reactor thanks to its excellent thermo-mechanical properties**[1]**. However, W is also known to have poor performance against irradiation damage. Its weakness comes from a lack of point-defect-controlling mechanism; specifically, the migration energy barrier of a self-interstitial atom (SIA) in unary W is extremely low.

Meanwhile, solute atoms in alloys can attract point defects and can change the mobility of them. In W-based transition metal binary systems, solute atoms such as Re prefers to make solute-SIA mixed dumbbell and migrates through the non-dissociative migration mechanism**[2]**. This non-dissociative migration mechanism raises the migration energy barrier up to some level. However, the migration energy gap between vacancy and interstitial remains still huge.

To control mobility of interstitial further, adding additional alloying agent is unavoidable. Thus, we chose W-Ta-Re system as the first ternary system to investigate, and, have conducted both energetics and dynamics analysis via first-principles calculations to find stable interstitial defect structure and check its mobility.

It is confirmed that, in such system, Ta and Re pair strongly attracts a W SIA, forming a Ta-Re-SIA triple complex. The interaction is stronger than that between Re and SIA in binary system. The strong interaction restricts the well-known non-dissociative migration motion of Re-SIA mixed dumbbell and effectively reduce the interstitial mobility. Reduced mobility in such ternary system can offer the increase in the odds of vacancy-interstitial recombination in collision cascades and the retardation of interstitial clustering.

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The analysis of pattern distortion in plasma etching process of silicon: Monte Carlo-based modeling and simulation

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Key Words: *Monte Carlo, High aspect ratio etching, Ion-assisted Chemical etching, Aspect ratio dependent etching, Feature size dependent etching, Pattern distortion, Silicon*

Abstract

In memory semiconductors for a high-aspect-ratio structure, it is common to observe shape distortion such as bowing and tilting in a plasma etching. Since this distortion leads to degradation of device performance, it is essential to analyse the cause based on an understanding of the etching process. In this study, the authors present a Monte Carlo (MC) based etching computational simulation technique by considering recoil atoms produced in the substrate via collision cascade after ion bombardment. We confirm the relationship between ion energy and etching amount in the ion-assisted chemical etching process through the number of recoil atoms [1]. The model also shows that the results qualitatively agree with well-known etching phenomena such as feature size dependent etching (FSDE) and aspect-ratio dependent etching (ARDE) [2].

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Virtual Dislocation Core Model for Dislocation Dynamics Simulation of Dislocation-precipitate Interactions

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Key Words: *Virtual Dislocation Core, Dislocation Dynamics, Dislocation-precipitate Interaction*

This paper presents a virtual dislocation core (VDC) model for dislocation dynamics (DD) simulation of dislocation-precipitate interactions. In the conventional DD method, dislocations are described as a curved line with a directional displacement jump equivalent to the Burgers vector. The elastic interaction between dislocations and the self-interaction can be accounted for in the calculation of the force acting on the dislocations. The force is then converted to the dislocation velocity based on a simple mobility (linear) law. However, in the DD method, the influence of the structural change in the dislocation core during the dislocation-precipitate interaction process cannot be considered. Takahashi et al. has proposed a DD simulation technique, which is an application of discretized Peierls-Nabarro model to the dislocation-precipitate interactions [1]. In the method, dislocations are discritzed with several fractional dislocations, and the dislocation core structure is described as the 2-dimensional planar arrangement of the fractional dislocations. The lattice restoring force arising from the difference in the generalized stacking fault energy in the matrix and the precipitate is changed according to the position of the fractional dislocation. The method can consider the influence of the structural change in the dislocation core, and however, the necessary computational cost is quite high. In addition, the numerical stability is also problematic due to the close interaction of fractional dislocations within the dislocation core.

In this study, a VDC model is proposed to enable us simulating the dislocation-precipitate interactions using the DD method with a realistic computational cost and high numerical stability. In the VDC, the dislocation core structure is locally defined as a 1-dimensional arrangement of virtual fractional dislocation (VFD) at the integral point along the dislocation segment. The VFD experiences the self-force and the elastic interaction force calculated in the DD method. In addition, the lattice restoring stress and the elastic interaction between VDC within the dislocation core are also considered. Thus, dislocations can be modelled as a single curved line, which drastically reduces the computational cost and improves the numerical stability compared to the DD simulation with full fractional dislocations. As a demonstration of the dislocation-precipitate interaction simulation using the VDC model, the γ-precipitate interaction with dislocation is simulated, and the critical resolved shear stress (CRSS) of the interaction is calculated. The CRSS calculated with the VDC model is comparable to that calculated using the DD method with the full fractional dislocations. Moreover, the dislocation shape and the core structure calculated with the VDC model are in good agreement with those calculated with the DD method with full fractional dislocations. The VDC model is further applied to the dislocation-sheared spherical precipitate interaction problem. The lattice restoring stress for the matrix, precipitate and the interface between the matrix and precipitate is used. The CRSS and the interaction mechanism are discussed in the paper.

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Activation barrier and critical stress of interactions between screw and edge dislocation with grain boundary in Cu

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Key Words: *Grain Boundary, Dislocation, Defect interaction, Nudged elastic band method*

It is well established that the strength and ductility of the polycrystalline metals are significantly influenced by the interaction between the dislocations and grain boundaries (GBs). Several representative phenomena are observed when the dislocation impinges the GB: 1) the dislocation is absorbed into the GB; 2) the dislocation transmits through the GB and slips on a certain plane in adjacent grains; and 3) the dislocations plie up before the GB, which imitates a wall or barrier to the movement of dislocations. Several factors can affect the interaction mechanisms and critical interaction shear stress (CISS), such as the local GB structure, GB energy, material elements, type of dislocations, and so on.

To investigate the influences of GB energy on the defect interaction, molecular dynamic (MD) simulations were performed for edge dislocation-<112> axis symmetric tilt GBs in Cu. It was found that the CISS would decrease when the GB energy increases if we only consider the weakest point alone the GB plane. Meanwhile, the interactions between a screw dislocation and coherent twin boundary (CTB) were implemented to interpret the material influence on the CISS in Cu, Al, Ni, Ag, Au, Pd. The CISS will be influenced by the difference between the unstacking fault energy and stacking fault energy.

Furthermore, as the dislocation-GB interactions were usually treated as the thermally activated process which could be accurately estimated by the transition state theory, we used the nudged elastic band (NEB) method to determine the saddle point and energy barrier of the interaction in a certain deformation state. It was found that the energy barrier would decrease when the shear stress increases because the high-stress state promoted the interaction and reduced the energy that should be externally introduced to trigger the interaction. The subsequently derived activation volumes ($13\sim31\,b^3$) and strain rate sensitivities corresponded well with the experimental data for the edge dislocation-<112>axis GB in Cu. A similar process was also applied to the screw-CTB interaction, the activation volumes and strain rate sensitivities corresponded well with the experiments. This process also quantitatively linked the MD to the realistic experiments.

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Alloy design from first-principles calculations of dislocation core in dilute and highly-concentrated alloys

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Key Words: *Alloy design, Mechanical Properties, Dislocation Core, First-principles Calculations*

Dislocation has been regarded as the essential lattice defect in plastic deformation, especially in metallic materials. The fundamental properties of the dislocation core have a dominant influence on the intrinsic ductility or brittleness of materials. The interaction between dislocations and other crystal defects plays a critical role in determining the mechanical properties of metals. The classical strengthening mechanism was developed by this central premise, and the mechanical properties of metals have been developed by understanding and controlling the dislocation behavior.

Especially, plastic deformation in BCC metals is achieved by a fundamental motion of screw dislocations through a kink mechanism. Alloy elements influence the mechanical properties significantly, where the classical strengthening mechanism can no longer be applied to the alloy design due to the complex effect derived from the electronic structure. The first-principles calculations have been widely applied to calculate the dislocation core of various metals directly. The core structure of dislocation in pure BCC metals and the effects of solutes on core structure have been investigated by the first-principles calculations. In the present study, we evaluated softening/strengthening behavior of dilute and highly-concentrated BCC alloys by the first-principles calculations. The introduction of dislocations within our periodic cell was accomplished by applying a continuum linear elastic theory solution for the periodic dislocation dipole array [1]. Then, we proposed new analytical models describing the kink process of screw dislocations, in which the fundamental properties are evaluated by the electronic structure calculations. The analytical models based on the solid solution and the line-tension model were applied efficiently to predict the fundamental mechanical properties. The first-principles calculations of dislocation core provided a clear trend in interactions between a solute and a screw dislocation depending on the type of alloying elements, revealing that the electronic structure around the dislocation core strongly influences the kink process. Furthermore, the analytical model reproduced the macroscopic solid solution softening/strengthening behavior in dilute alloys and the unique slip behavior in highly-concentrated alloys.

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Atomistic Investigation of Hydrogen Influence on the Mobility of Edge Dislocations in Alpha-Iron

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Key Words: *Edge dislocation, Molecular dynamics, Alpha iron, dislocation mobility, Hydrogen concentration*

It is worthwhile to investigate the interplay between impurities and dislocations in metals from both a basic and a practical standpoint since there are several intriguing topics to consider. In a crystal, impurity atoms, complexes, and impurity clusters scattered throughout the crystal all have an effect on the mobility of dislocations via a variety of mechanisms. In this study, we use extensive molecular dynamics (MD) calculations, based on a highly-accurate interatomic potential to examine how hydrogen atoms impact the mechanisms behind the mobilities of edge dislocations in body-centred cubic (bcc) alpha-Iron (α -Fe) at a temperature ranging from 300 K to 500 K. The edge-dislocation mobility in α-Fe is shown to be temperature and hydrogen concentration-dependent in this MD investigation. It is demonstrated from the results that hydrogen impurities that are efficient in locking dislocations exist in the form of complexes that are scattered discretely along the dislocation line and that these complexes operate as extremely effective impediments to the mobility of edge dislocations. The hydrogen impact on the edge dislocation motion from the dislocation velocities versus shear stress reveals that the movement of edge dislocations in α-Fe with Hydrogen is much damped as the hydrogen concentration increases. Increased hydrogen concentration produces internal strain in the α-Fe cristal; hence, the shear stress increases with decreasing dislocation mobility. According to the atomistic structure study results, when the dislocation velocity is very low (less than 1 m/s), the movement of Hydrogen atoms with the edge dislocation segment is enhanced because the longer time is given for Hydrogen to catch up the dislocation motion. Therefore, the synchronized motion of the Hydrogen and dislocation segment is increased with decreasing dislocation velocity. Furthermore, the drag coefficient calculated from the dislocation velocity vs stress graph reveals that it decreases with temperature in α-Fe containing hydrogen atoms. As the temperature decreases, it is clear that Hydrogen has a more significant influence on edge-dislocation mobilities with increased shear stress, as seen by the data. Even with small cell size, a unique locking mechanism is identified in the α-Fe, which increases the necessary stress for dislocation migration in α-Fe. Specifically, our studies indicate the prominent processes of edge-dislocation motion in α-Fe, as well as particular implications of temperature and Hydrogen on these mechanisms, all of which have the potential to have a considerable influence on the mechanical properties of α-Fe. As a result of this research, it is concluded that temperature and hydrogen concentration is very significant determinants of deformation in hydrogen-containing metals since much lower temperatures are used for Hydrogen storage applications [1,2].

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Atomistic Modelling of Fracture in iron via Gaussian Approximation Potential

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Key Words: Fracture, Iron, Interatomic Potential, Machine Learning

Predicting fracture of iron-based alloys (steels) as a function of alloying/chemistry and loading conditions is crucial to optimize their mechanical performance for many applications. Fracture is controlled by multi-scale mechanisms that originate at the atomistic scale. Therefore, understanding fracture of pure iron at the atomistic scale is essential to build a predictive model of fracture for iron-based alloys.

Molecular dynamics (MD) is a suitable tool to explore atomistic mechanisms occurring at crack tips. The reliability and accuracy of MD depends on the interatomic potential (IAP). Many Fe IAPs have been published, but none of them is capable of reproducing the experimental evidence of fracture in iron [1]. Here, we develop a new Gaussian Approximation Potential (GAP) for fracture in iron, by extending a previous Fe GAP [2]. We enrich the existing density function theory (DFT) database [3] by adding crack-relevant configurations, including highly deformed primitive cells and surface separation.

The new Fe GAP preserves DFT-accurate properties (elastic constants, surface energies, and Bain path). Together with other state-of-the-art IAPs, mode-I fracture process of single-crystal iron is studied for several crack fronts and planes, by performing molecular statics. The cleavage plane and critical stress intensity factor are compared with experiments and with Griffith theory. The competition between cleavage on $\{100\}$ and $\{110\}$ planes is studied and simulations, theory, and experiments are compared. Our study provides a systematic strategy for improving machine learning IAPs for fracture.

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Atomistic Simulation of Nano-scale Drawing of Metallic Wires: Comparison on Plasticity Process between Fe and Mg Materials

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Key Words: *Wiredrawing, Plastic deformation, Iron and steel, Magnesium, Molecular Dynamics*

Wiredrawing is a conventional method for plastic working to make wires narrower and it has been applied to wide variety of metallic materials. Industrial needs for smaller sized wires, such as those with micro-meter or nano-meter size dimension, are now continuing, whereas there is no clear insight of the wiredrawing when the process size comes to such an extremely narrow region. This study aims to acquire the possibility of fabrication technique of very small wires and to establish the theoretical foundation concerning wiredrawing process in nanometer-sized region. Contrast to conventional simulating method based on finite element analysis (FEA) which has been already widespread in industry, molecular dynamics (MD) analysis (atomistic simulations) will become a central methodology to investigate the process in near future.

So far, material models of pure iron (Fe) and pearlitic steel which contains carbon atoms as well as Fe atoms are well established by the present authors [1], and theoretical prediction concerning plastic deformation mechanism and atomic processes in drawing of Fe-based materials has been paid attention. Recently, our simulations are going to be applied to pure-magnesium (Mg) nanometer-sized wire. The Mg material contains well-known difficulty in any cold plastic working due to restriction of slip systems inherent to hexagonal closed-packed (h.c.p.) structures. We will compare our previous results of plastic process in wiredrawing of Fe-based (body-centered cubic: b.c.c.) material [1] with h.c.p. wires.

In the simulation of metallic wire, a conical die with semi-angle of 7 degrees is spatially fixed and the wire passes through the die with a given drawing speed. Since intact interaction energy between die and wire atoms offered by EAM potential function is tremendously large, the interaction for pairs in the vicinity of the interface is adequately reduced by modifying the strength. Simultaneously, the wires are subjected to plastic strain which is needed for the reduction ratio of the diameter. By using wire models made of Mg single crystal with various crystal orientations, it is found that deformation twinning works very effective for accumulation of the plastic strain. On the other hand, it is observed that slip systems inherent to Mg crystal are fatally limited in contrast to pure Fe crystal, as crystallographically predicted. We can observe atomistic processes of formation and propagation of twin planes, basal slips and their combination, which are unique to the Mg crystal. Interestingly, deformation twins are followed by phase transformation from h.c.p. phase to b.c.c. phase. It is concluded that nanometer-sized wiredrawing is theoretically possible for the Mg material, but deformation process there is totally different from Fe-based material and drawing orientation strongly affects the plasticity. Therefore, we can suggest that a selective condition of wiredrawing certainly exists for Mg in any size-scale.

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Automated Atomistic Analysis of Interfacial Dislocations and Disconnections: Application to Martensitic Transformations

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Key Words: *Dislocation, Disconnection, Interface, Molecular Dynamics, Martensitic Transformation*

Line defects like dislocations and disconnections play critical roles in the thermodynamics and kinetics of interfaces in crystalline solids; the Burgers vector content of the defects accommodates mismatch and misorientation across the interface, while the step character of disconnections enables migration of the interface via their glide motion. While the continuum perspective on interfacial line defects has greatly matured in recent years thanks largely to the development of the topological model by Pond and Hirth [1], atomistic analysis of interfacial line defect structures is still in its infancy. This is largely due to the difficulty of identifying and characterizing interfacial line defects in atomistic datasets. While the revolutionary dislocation extraction algorithm (DXA) tool can automatically identify interfacial dislocations, it requires the specification of an atomic motif for the interface structure [2,3]. This is labor-intensive and often difficult to accomplish in practice. Furthermore, DXA cannot identify disconnections. Building on the success of DXA, we develop a new technique for identifying interfacial line defects which is based on the concept of constructing Burgers circuits between coincidence sites in the interface. This technique does not require any structural input about the interface and can identify both interfacial dislocations and disconnections. Using this new technique, which we call the dislocation and disconnection extraction algorithm (DDXA), we analyze interfacial migration during martensitic transformation in Fe, revealing the key interplay between bulk and interfacial line defects.

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Description of hardening behaviour with slip transfer across grain boundaries of bicrystals using crystal plasticity FEM

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Key Words: *Crystal plasticity, Grain boundary, Bicrystal, Hardening with slip transfer, Dislocation density, Finite element analysis*

Precise prediction on strength of polycrystalline materials needs the knowledge of hardening behaviour with slip transfer across grain boundaries (GBs). In this study, plastic deformation near GB of bicrystal was numerically analized using crystal plasticity finite element method (CPFEM). To describe the hardening behaviour by CPFEM, a constitutive equation based on Kocks-Mecking model [1] with slip transfer effect across GB was proposed and implemented by using a user material subroutine of LS-DYNA. For the description of GB interaction, the geometrically necessary dislocation (GND) density near GB induced by strain gradient was affected by the transmission factor representing the degree of slip transfer across GB. In the present model, the factor is based on a criterion considering the intersection between slip plane and GB proposed by Shen et al. [2]. To discuss the validity of the introduced GB model based on CPFEM, two models were considered; one is a bicrystal subjected to uniaxial tension normal to GB and the other is one subjected to simple shear perpendicular to GB. The former is for numerical verification comparing with the reference [3], and the latter for that to the GB interaction criterion. The preferential slip system across GB and the plastic deformation near GB were especially discussed for several kinds of GBs of aluminium bicrystals.

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Effect of cross-section shape on critical resolved shear stress of crystal slip in nanorods: A molecular dynamics study

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Key Words: *Nanoscale, Schmid's law, Dislocation*

The mechanical properties of nanoscale metallic materials differ from those of bulk materials because of lack of dislocation sources inside the materials [1] and the increased influence of surfaces [2]. For example, Cao *et al*. indicated by molecular dynamics (MD) simulation that the yield stresses differ between quadrangular prism and cylinder nanorods of Cu single crystal with the same crystal orientation [2]. In the case of bulk materials with the same crystal orientations, the yield stress is independent of the cross-section shape and the critical resolved shear stress, τ_{CRSS}, is constant (Schmid's law). The research by Cao *et al*. suggests in contrast that Schmid's law may not hold in the nanoscale materials. However, the effect of surface orientations and edge between them, which should play a vital role in slip occurrence in nanorods, has not been clarified.

In this study, we performed a uniaxial tensile deformation simulation using MD for Cu single crystal nanorod models in which the cross-section shape was systematically changed. To evaluate the basic slip deformation, we set a crystal orientation of the nanorods so that the slip of the specimen under the uniaxial tensile load becomes a single slip. The cross-section shapes of the nanorods were square (Sqr), square rotated by 45 degrees (Sqr45), regular octagon (Oct), and circle (Cir). The length of one side of Sqr and Sqr45 models and the diameter of Cir model were 20 nm, and the length of one side of Oct model was 8.28 nm. The lengths in the loading direction of all models were 34 nm. With the periodic boundary condition only along the loading direction, we conducted MD simulation at 300 K to evaluate the slip deformation and calculate τ_{CRSS}.

In the Sqr, Oct and Cir models, the deformation occurs only in the main slip system, and the τ_{CRSS} of each rod was 1.34, 1.59 and 1.69 GPa, respectively. On the other hand, although the crystal orientation is the same as that of the other models, the deformation in the Sqr45 nanorod occurs in the second slip system and the τ_{CRSS} is 1.00 GPa. These results indicate that the cross-section shape remarkably affects the slip deformation and that Schmid's law does not hold in the nanoscale materials. To investigate the effect of surface edge on the slip deformation, we also conducted MD simulation for nanorods with varying chamfers in square. We will discuss the detailed mechanism in the presentation.

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Effects of Dynamic Segregation on Grain Boundary Migration in High-entropy Alloys

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Key Words: *High-entropy alloy, Molecular dynamics, Grain boundary, Segregation, Solute-drag*

High-entropy alloys (HEAs), which are solid solution materials obtained by mixing more than five elements with near equiatomic fractions, have attracted significant attention because of their excellent mechanical properties such as thermal stability at high temperatures [1]. The excellent thermal stability of HEAs needs to suppress the activation of grain boundary (GB) migration that causes grain growth. Hence, understanding a detailed atomic behavior at GBs in HEAs is indispensable to elucidate the mechanism realizing the thermal stability of HEAs. Elemental segregation to GBs, where equiatomic fraction breaks, have been reported in HEAs [2]. This suggests that dynamic GB segregation and drag of atoms might occur when the migration of the GBs is sufficiently slow. These dynamic phenomena could increase a driving force required for the continuous GB migration. However, it is not easy to capture the dynamic behavior of atoms using only experimental approaches. In this study, we investigate the influence of the dynamic GB segregation on the GB migration in HEAs through molecular dynamics (MD) simulations.

Equiatomic FeNiCrCoCu-HEAs with a Σ17(530)[001] high-angle tilt GB is modeled with interatomic interactions developed by Farkas *et al* [3]. The GB is moved by an applied shear strain parallel to the GB plane. In this study, we investigate GB velocity dependence of GB migration through controlling shear strain rate. These simulations are performed at $T = 0.85\ T_m$, where $T_m = 2090$ K is melting temperature of the HEAs. For the comparison with HEAs, we conduct the same analyses with an interatomic potential of pure Cu developed by Mishin *et al* [4].

The GB migrates at various velocities from 0.07 m/s to 15 m/s under different driving forces. In pure Cu, the relation between the GB velocity and the driving force is almost linear. The HEA also exhibits the same linear relation, but the susceptibility of the GB velocity to the driving force in the low GB velocity region significantly smaller than that in the high-velocity region. We confirm dynamic GB segregation occurs in the low-velocity region. The effect of the segregation on the GB migration could be explained in terms of the reduction of atomic diffusion at GBs because the GB migration requires atomic rearrangements at the GBs which would be reflected in the atomic diffusion. To examine the effect of GB segregation on GB migration, we compare the activation energy of the atomic diffusion under no external load between two types of GBs; a GB where the elements are assigned randomly and a GB where the elements are assigned closely to thermal equilibrium obtained by a hybrid procedure of Monte Carlo and MD simulations. The later GB distribution mimics the composition of the dynamically segregated GB. The activation energy of diffusion in the thermally equilibrated GB is higher than that in the randomly assigned GB. Therefore, the dynamic GB segregation increases the energy barrier for GB diffusion, which can be related to an increase in the driving force required for the GB migration at lower velocities.

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Energetic Analysis of Homogeneous Nucleation of $\{10\bar{1}2\}$ Twin in Magnesium

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Key Words: *Deformation Twin, Nucleation, Magnesium, Nudged Elastic Band Method*

Magnesium has attracted much attention from engineering viewpoint because of its low density and relatively high specific strength. At room temperature, magnesium has only the major slip systems of basal slip and non-basal slips are difficult to be activated. Deformation twinning is an essential mode of plastic deformation. There are two typical modes of twinning. While the critical resolved shear stress (CRSS) for the $\{10\bar{1}1\}$ compressive twinning is high, the $\{10\bar{1}2\}$ tensile twinning has low CRSS and appears in an early stage of plastic deformation, related to the low dislocation energy and the low Peierls barrier of $\{10\bar{1}2\}$ twinning dislocation [1]. Although $\{10\bar{1}2\}$ twins are considered to generate preferentially from inhomogeneous regions associated with grain boundaries and dislocations [2], understanding homogeneous nucleation of twins gives us fundamental information on $\{10\bar{1}2\}$ twinning. In this study, we energetically evaluate homogeneous nucleation of $\{10\bar{1}2\}$ twin using the nudged elastic band (NEB) method. The NEB analyses of homogeneous twin nucleation under shear strain are carried out and the shear strain dependence of the activation energy barrier is discussed. The NEB results are compared with a simple nucleation model.

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First-principles prediction of short-range ordered structures of solute atoms during aging in Al-Mg-Si alloys

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Key Words: *Al alloys, Aging, Solute cluster, Density functional theory, Monte Carlo method*

Al-Mg-Si alloys are widely used in the automotive and aeronautical industries because of their excellent properties, including high strength-to-weight ratios, good formability, and high corrosion resistance. The hardness of the alloys is increased through aging, in which the formation of solute clusters and metastable precipitates hinders the motion of dislocations. During precipitation of Al-Mg-Si alloys, solute atoms diffuse and aggregate to form nanosized clusters while maintaining coherency in the matrix. Then, the metastable β" phase, which is the main strengthening phase of the alloys, begins to nucleate as the clusters grow. Because the strength of the alloys changes significantly depending on the temperature during aging [1], solute clusters formed before nucleation of the β" phase are believed to affect the resultant strength of the alloys. Therefore, identifying the specific process involved in the short-range ordering of solute atoms during aging is essential in controlling the mechanical properties of this alloy system and in designing new alloys with superior performance. A previous experimental study [2] revealed that the compositions and thermal stabilities of solute clusters in Al-Mg-Si alloys changed dramatically depending on temperature. However, the details of the atomic structures of solute clusters have yet to be clarified.

In this study, we evaluated the interaction energies between solute atoms and vacancies in the Al matrix using first-principles calculations and constructed a multi-body potential for the Al-Mg-Si system. Atomistic Monte Carlo (MC) simulations were then performed to analyze the formation behaviors and thermal stabilities of solute clusters. Equilibrium MC simulations without detailed balance [3] were conducted to simulate the thermal equilibration of the Al-Mg-Si system under various temperatures. Results indicated that the temperature range in which the solute clusters were formed was limited, and the sizes and compositions of the clusters changed temporarily with temperature. At low temperatures, the sizes of the clusters were relatively small and their compositions were widely distributed from Si-rich to Mg-rich. In addition to many small Si-rich clusters, Mg-Si or Mg-rich clusters with $L1_0$-type ordered structures were formed. However, at high temperatures, the sizes of the clusters were relatively large and their compositions asymptotically approached Mg/Si = 2 (i.e., Mg-rich) as the cluster size increased. The Mg-rich clusters formed at high temperatures also had internal $L1_0$-type structures. We found that Mg-Si or Mg-rich clusters that were initially formed under low temperatures grew under higher temperatures, whereas Si-rich clusters maintained their sizes and compositions during MC sampling. Our results on the relationship between cluster size and Mg/Si ratio were consistent with those of the experimental counterpart [4]. Our study provides a modeling approach that efficiently uses first-principles-calculated energies and an MC model in a scale-bridging manner to elucidate the thermodynamic characteristics of the formation of solute clusters.

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FTMP-based model for the Bauschinger effect on FCC metal

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Key Words: *Field Theory of Multiscale Plasticity, Inhomogeneity, Bauschinger effect, Crystal plasticity, Strain gradient plasticity, Finite element method*

INTRODUCTION

The Bauschinger effect intrinsically involves multiscale problems of complex kinds when it comes to its rational modeling beyond phenomenological approaches that rely on kinematic hardening laws, despite being one of the classical issues in plasticity. The associated transient and permanent softening behaviors, including apparent reduction in the elastic moduli as well as the early re-yielding phenomena, stem strongly from deformation-induced inhomogeneous fields to be developed in plural scales, e.g., intra-granularly evolving dislocation substructures and those associated with inter-granular nonuniformities.

The present study intends to tackle this issue from the persepctive of evolving inhomogeneous fields that naturally bring about irreversibilities during load reversal based on Field Theory of Multiscale Plasticity[1] (FTMP). FTMP allows us to reproduce dislocation substructure evolutions in single crystals, simply by additively introducing the incompatibility tensor-based defect degrees of freedom in an appropriate manner in the hardening law to be used.

CONDITIONS

We extend such series of simulations to polycrystal models under tension-compression straining, with 163, 613, 1351, and 2377 grains, respectively, by allocating six typical orientations of $(100)[001]$, $(110)[001]$, $(100)[011]$, $(\bar{1}\bar{1}0)[\bar{1}10]$, $(1\bar{1}0)[111]$, and $(11\bar{1})[123]$ randomly to them, where the intragranular substructure evolutions are simulated simultaneously.

RESULTS AND CONCLUSION

The transient softening tends to appear even in the 163 model and is shown to be enhanced with increasing number of grains, while the permanent softening seems to require sufficent number of grains for it to naturally emerge. Contributions from intra and inter-granular inhomogeneities are examined by carefully separating each by taking differences among simulation results obtained under selected conditions with and without the incompatibility models.

At the same time, the associated energy conversions from elastically-stored states to local plastcity measured by variations of the incompatibility is scrutinized based on duality diagram representation scheme, where the diagram is constructed by plotting the incompatibility trace against the fluctuation of the elastic strain energy. SThe ratio of the ordinate to the abscessa of the diagram at the maximum tension, referred to as duality coefficient, representing the energy conversion rate, is demosntrated to correlate well the Bauschinger strain, as a measure of transient softening. This eloquently implies that the irreversibilities causing transient softening stem majorly from the inhomogeneous fields evolved during the forward loading.

The comparison among the four models is further made to systematically examine the effect of inter-granular inhomgeneities on the transient softening.

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FTMP-based Series of Simulations on Kink Deformation/Strengthening In Mille-feuille Structured Mg

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Key Words: *Mille-feuille structure, Kinking, Crystal plasticity, Finite element analysis, Single crystal, Elastic energy*

Kink-strengthening for mille-feuille structures has attracted many attentions in recent years. This study aims at identifying the kink formation/strengthening mechanisms via numerical reproductions of emerging kink-like morphologies. Reproducing ridge kink morphologies and the attendant strengthening for a single crystal Mg model are explored based on CP-FEM devised with FTMP (Field Theory of Multiscale Plasticity). In FTMP, defects in a crystal are considered as torsion and curvature, and these are calculated as dislocation density tensor and incompatibility tensor in continuum mechanics. By introducing these two into the hardening ratio in the hardening development law, the theory can reproduce the heterogeneous deformation inside the material. The incompatibility tensor-based relevant underlying microscopic degrees of freedom satisfying rank-1 connectivity condition, referred to as "kink model," is introduced either explicitly or implicitly to the conventional slip-based constitutive framework. The use of the explicit model exhibits realistically-resembling ridge kink morphologies. The energy release associated with the kink also approximates the results observed in experiments. whereas the implicit model allows raised stress response accompanied by relatively heterogeneous kinking structures, provided appropriate initial imperfections as well as mille-feuille structures that can effectively store excessive elastic strain energy. We have predicted that the mechanism of kink generation is the mutual exchange of energy stored in each of the hard and soft layers. The simulation results described above include an experimentally-observed unique feature reported based on the AE (acoustic emission) technique, demonstrated to exhibit power-law type distributions both in the strain energy fluctuation and the incompatibility from the early stage of deformation even before the massive emergence of kink-like regions, analogous to the AE observations. They lead us to tentatively conclude that the layered structure associated with the incompatibility-based relevant degrees of freedom, in addition to a sufficient constraint of the basal slip activity, can play pivotal roles in reproducing the targeted feature. Extended discussions of all the above are further made via the corresponding duality diagram and scale-free representations. Also demonstrated is a successful reproduction of the peculiarly-deformed specimen under slightly-inclined tension experimentally observed recently, shown to brought about by kinking deformation as well. This further backs up the validity of our simulation model.

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Influence of Interface Properties and Misfit Dislocation Networks on The Stress Fields in Multilayered Material

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Key Words: *Multilayered Materials, Misfit Dislocation Networks, Interface Properties*

Anisotropic multilayered materials in a nanoscale thickness have been applied to the electronic devices such as a semiconductor, sensors, MEMS and NEMS. Misfit dislocation networks frequently occur at the interface in multilayered structures composed of different crystal structures. Furthermore, atomic structures near the interface are different from each bulk structure. The interface energy occurs in a similar manner to the surface energy[1]. Then, the interface energy can be expressed a function of surface strain. The interface stresses and interface elasticity originated from the atomic structures near the interface are calculated from the first derivative and the second derivative of the interface energy with respect to the interface strain. In the present paper, the interface properties, such as the interface stresses and interface elasticity, are obtained using the molecular statics analysis. On the other hand, stress and displacement fields for the multilayered structures with misfit dislocation networks are deduced using a three-dimensional Stroh's formalism[2][3]. Until now, the transfer matrix method was usually applied for analyzing the stress and the displacement around a misfit dislocation at the interface in the multilayered materials[4]. When the interface properties are taken into the boundary condition at the interface, the transfer matrix method cannot be used. So, a new method is needed to develop for the analysis. Furthermore, when the boundary conditions for the top surface and the bottom surface are prescribed, the unknown vectors using in the displacement and traction expressions become very complicated. In the present analysis, a simplified expressions for the unknown vectors including all boundary conditions, such as the interface properties, are deduced through some recursive formulae of the *m*-th layer. Then, the expressions for displacement and traction for arbitrary number of layer could be explicitly deduced. The procedure for the expressions can be extended to isotropic materials. The interaction of misfit dislocation networks existing at different interface is investigated and also the influence of the interface properties on the interaction is clarified. The stress and displacement fields for the derived solutions are compared with those obtained by the molecular statics analysis to demonstrate the validity of the solutions.

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Investigation of interaction between dislocations and obstacles in BCC iron by using neural network atomic potential

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Key Words: BCC iron, Dislocation, Obstacle, neural network atomic potential

Interaction between dislocations and obstacles, such as void and precipitates are important in the strength of BCC iron. Because of size of dislocation core which is typically less than 1 nm, the investigation of the interaction between dislocations and obstacles requires the use of atomic modeling. Because of long range elastic interaction of dislocations, atomic modeling for dislocation dynamics require usually 100,000$\sim$ atoms. Therefore, usually, empirical atomic potentials, such as embedded atom method (EAM) are used for investigation of dynamic interactions between dislocations and obstacles. However, the predicted structure and energetics of the dislocation core by empirical inter-atomic potentials are not consistent with the results of first principles calculations based on density functional theory (DFT). Thus, the exact details of the interaction between dislocations and obstacles are still obscure. To overcome this problem, we constructed the atomic potential with DFT accuracy based on an artificial neural network (ANN) framework. [1]. In this research, by using the ANN potential, to investigate the interaction between edge dislocation and obstacles, we performed 1000,000 atoms molecular dynamics simulation with DFT accuracy.

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Investigation of local stiffness inside Ti_3AC_2 (A = Al, Ga, In) MAX phase using first-principles atomic stress calculation

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Key Words: *Local stiffness, MAX phase, First-principles calculation, Atomic stress*

In recent materials science, controlling heterogeneity, where different microstructures coexist in a single material, has been regarded as a fundamental strategy to achieve both strength and durability in structural materials. The elastic state is also spatially inhomogeneous in such structures; however, any computational method has not yet been established to reveal such an inhomogeneous elastic state at the atomic level.

We have developed a local stiffness calculation scheme based on the first-principles atomic stress calculation [1][2] and have applied this method to the MAX phases, Ti_3AC_2 (A = Al, Ga, In), which possess an atomic-level stacking structure (Fig. 1). As shown in Table 1, the computational results obtained by this scheme properly represents the difference between the soft layer (Ti-A-Ti) and the hard layer (Ti-C-Ti-C-Ti) inside the MAX phases. In the presentation, we will discuss the details of the local stiffness calculation and the electronic structure of the MAX phases behind their local stiffness.

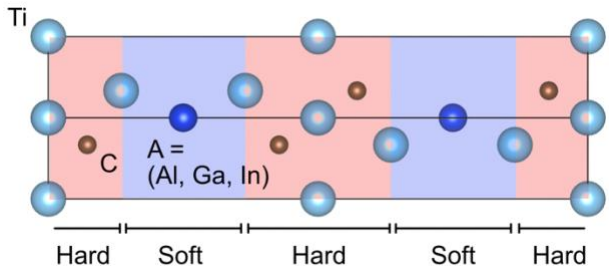

Fig. 1: Layered structure of Ti_3AC_2 MAX phase.

Table 1: Local stiffness [GPa] of Ti_3AC_2.

A	Layer	C_{11}	C_{33}	C_{44}
Al	Hard	427	335	133
	Soft	315	304	129
Ga	Hard	427	393	149
	Soft	311	262	119
In	Hard	398	362	137
	Soft	300	227	92

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Micropillar compression simulation of single crystal materials based on FTMP

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Key Words: *FTMP, Compression test, Plastic deformation, Slip, Dislocation, Simulation*

This study attempts to clarify a sort of an application limit of FTMP (The Field Theory of Multiscale Plasticity) [1] in describing semi-discrete microscopic processes of dislocations, through a systematic series of simulations on micropillar compressions against single crystal samples. Micropillar tests [2] have been recently attracted attentions as a direct measure to tangibly investigate mechanical properties of materials in micrometer regions, and have been further extended to nanometer regions. The marked features include intermittent as well as isolated nucleation and expansions of dislocation loops generated from a limited number of sources that are statistically pre-existed within the sample to be tested, resulting in extremely high yield stress followed by strain bursts with eventual terminations due to source starvations [3], leaving finely and massively stepped surface morphologies through which dislocation loops had been passed away. FTMP, on the other hand, possessing prominent descriptive capabilities for deformation-induced inhomogeneities of evolving kinds, has been demonstrated to enable crystal plasticity-based finite element (CP-FE) simulations to easily and naturally reproduce dislocation substructures with various morphologies and the associated misorientation developments, simply by adding the incompatibility tensor-related appropriate defect degrees of freedom to the hardening law being employed,[1] and recently has been successfully applied also to "kinking" related stuff in Mg, including both their formations and contributions to the strengthening. Here, we perform some preliminary approaches aiming at reproducing the above features, assuming a 2D single crystal sample with nearly ideal strength, equipped with a few regions having high Schmid factor, as a source of dislocation generations. Demonstrated tentatively are expanding dislocated regions at the onset of the first strain burst, as well as the resultant emergence of surface steps. The results are further examined in detail by visualizing the energy transfer from elastically-stored states to local plasticity via the variation of the incompatibility field, by using duality diagram representation scheme, where the diagram correlates the trace of the incompatibility tensor with the fluctuation of the elastic strain energy. There observed an abrupt increase in the incompatibility with strain energy fluctuation nearly unchanged at around the onset of the strain burst, representing a nucleation of a set of dislocations from one of the introduced source regions. The completion of the present study will greatly extend the wing of the possibilities of continuum mechanics-based top-down approach toward micro-plasticity.

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Modeling and Numerical Analysis of Screw Dislocations based on Differential Geometry

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Key Words: *Screw Dislocation, Size Dependent, Differential Geometry, Finite Element Method*

In this research, we investigate the size dependent elasto-plastic deformation of screw dislocations in a nano-scale object. Our method is based on the continuum mechanics on the Riemann-Cartan manifold [1-3]. This mathematical framework introduces the three different configurations, reference R, intermediate B, and current S configurations, in order to express the elasto-plastic deformation. Here, the first map, from R to B, represents the plastic deformation and the second one, from B to S, corresponds to the elastic relaxation. The total deformation gradient is expressed by the multiplicative decomposition of the respective deformation gradients: F_p and F_e.

For a given distribution of the dislocation density, we solve the weak form of Cartan first structure equation to obtain the plastic deformation gradient F_p and Riemannian metric of the intermediate state B. The elastic deformation gradient F_e is then obtained from the minimization of strain energy functional. Note that, from a mathematical viewpoint, the elastic deformation is understood as the embedding of the Riemann-Cartan manifold into the conventional Euclidean space. We solved the variational problems numerically using the finite element method.

We investigated the stress and displacement fields of screw dislocations in a three-dimensional rectangular bar with the aspect ratio 1:1:10. Size of the bar is in the order of nano meters. The first model includes a single screw dislocation whose Burgers vector and dislocation line is set parallel to the longitudinal direction. Present numerical analysis revealed that the stress fields show no singularity even at the dislocation core. Deformation fields showed novel twisting phenomenon, which is called Eshelby twist, and the magnitude showed notable size dependence. That is, magnitude of the twisting angle increases monotonically with decreasing the size. The second model includes five twist boundaries along the longitudinal direction. Here, each boundary includes a pair of screw dislocations whose dislocation lines cross perpendicular in the boundary planes. Numerical analysis showed similar twisting as well as the size dependence of deformation. We will discuss the similarity of the two different configurations of screw dislocations from a view point of the differential geometry.

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Molecular dynamics study of stress generation in a DLC film deposited on Fe substrate

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Key Words: *Diamond-like Carbon, Deposition Process, Residual Stress, Mechanical Property, Molecular Dynamics*

Diamond-like carbon (DLC) film has superior tribological properties such as low friction and high wear resistance. However, one of the major problems with DLC films is the delamination during operation, which reduces the adhesion strength. High residual stress inside the film is reportedly one of the causes of DLC film delamination [1]. Thus, it is essential to elucidate the mechanism of residual stress generation in a DLC film during deposition. Numerical simulation studies for such mechanism are indispensable [2] as the experimental measurement of residual stress is challenging.

Recently, we elucidated through molecular dynamics (MD) simulations the residual stress mechanism in a DLC film during the deposition of carbon on a diamond substrate [3]. We performed the MD simulations using LAMMPS, which is a free and open-source software for classical molecular dynamics. Here, we found that the compressive stress in the film is caused by the structural change from sp^2 to sp^3 during the deposition process. As the bond length of sp^3 structure is larger than that of sp^2, the structure transition from sp^2 to sp^3 and the growth of sp^3 cluster causes the compression stress in the film.

In this study, the deposition processes of carbon on an Fe substrate were simulated by MD using LAMMPS. We compared the results with our previous work with a diamond substrate [3] to investigate the effect of substrate material on the stress generation in the DLC film.

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Multiscale modeling simulation of nano-micro metal fatigue

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Key Words: *Molecular Dynamics, Rate Equation Approach, Inverse Analysis, Machine Learning, Dislocation*

While the fatigue mechanism in macroscopic metal materials is well described by self-organization of dislocation structures, presumably such a description can no longer account for fatigue in nanometer- or submicron-sized materials because the dimension of a specimen is smaller than that of slip bands consisting of dislocation structures [1,2]. The fatigue mechanism of materials with nanometer or submicron dimensions, which we call "nano-micro fatigue", has been little understood, urging establishment of theories to explain the mechanism.

To tackle this fascinating but challenging problem, we are performing multiscale simulations covering the atomistic, mesoscale and micrometer scale levels. We first discuss atomistic model simulation with molecular dynamics (MD) of single crystal nano-sized metal models to observe dislocation behaviors under monotonic and cyclic loading. In a MD simulation of nanofilms under cyclic loads, we found slip localization when the initial structure contained distributed vacancies while slip deformations were almost evenly distributed in a pristine model, indicating an increased fatigue strength in nanometer-sized specimens where few defects are expected. We also performed a MD simulation of nanorods to find some peculiar behaviour at the nanoscale; e.g., activation of different slip systems depending on the temperature, nontrivial effects of surface edge structure on slip behavior, etc.

We are also performing simulation of dislocation structure formation by means of the rate equation approach, which solves differential equations of the development of density distributions of mobile and immobile dislocations under mutual interactions [3]. Using a thin film model, we confirmed that certain combinations of input parameters such as dislocation diffusivities and mobile-immobile dislocation interactions produce formation of aligned dislocation density peaks with certain distances between them, which is indicative of the dislocation wall structure. Whether the formation occurs and the dislocation structure (e.g. distances between dislocation walls) depend on the parameters. As it is difficult to determine the parameters for the phenomenological model, we constructed an artificial neural network (ANN) model to map between input parameters of a simulation method and output simulation results, which enables us to find parameters that result in realistic dislocation structures observed in experiment.

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Phase-field simulations on temperature-related behaviors of skyrmions: Topological defect dynamics

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Key Words: *Skyrmions, Phase-field model, Temperature, Topological defect, thermodynamics*

Controlling static and dynamic behaviors of the bubble-like magnetic skyrmion exhibits great potential in the application of spintronics. Especially, as a natural property, temperature plays an important role in the control of skyrmion behaviors. For example, statically, the temperature can lead to the phase transition of the topological magnetic structures (such as skyrmions) by affecting their stability; dynamically, fluctuated or inhomogeneous temperature fields can drive the skyrmion motion. However, due to the limitation of existing hypothesis-based simulation methods, the study of temperature-related behaviors of skyrmions from the perspective of thermodynamic free energy is rare. Here, we developed a temperature-related phase field simulation to predict and explain the skyrmion behaviors in temperature fields. Statically, we demonstrate the skyrmion lattice of a room-temperature ferromagnetic thin film lose the thermal stability near the 340 K, and obtain the temperature-magnetic field-strain phase diagrams of topological structures in MnSi thin film, which consists with the experimental results very well. Dynamically, we study the rectilinear motion of the individual asymmetrical skyrmion driven by temperature gradients, i.e., acceleration and deacceleration of skyrmions, and propose a kinematic equation to describe it. Therefore, our work demonstrates the temperature-related phase field simulation is a reliable method to simulate the skyrmion behaviors in temperature fields, and propose the thermodynamics explanation on both static and dynamic features of skyrmions, which is anticipated to be the theoretical support for further research about temperature-related behaviors of skyrmions, i.e., elementary development of topological defect dynamics, and their potential applications in functional devices.

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Reproduction Method of Mechanical Anisotropy Induced by Cold Rolling in Crystal Plasticity FE Simulation

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Key Words: *High entropy alloys, Crystal plasticity, Finite element analysis, Rolling texture, Mechanical anisotropy*

The crystal plasticity FE analysis considering the microscopic information describes the mechanical response of polycrystalline metals at the grain level. When the crystal orientation information of the actual material is applied to the analytical model for the crystal plasticity FE analysis, the crystal orientation is often randomly extracted from the EBSD measurement data. The number of crystal grains in crystal plasticity FE analysis is limited to a small number compared to the actual crystalline metals due to the problem of calculation cost. The conventional method of randomly selecting the crystal orientation does not reproduce the analytical model, and it results in significant variations in the analytical results depending on the combination of crystal orientation. It is essential from the viewpoint of computational cost to reproduce the crystal orientation distribution of the actual material in an analytical model with a small number of grains.

In addition, the rolling texture induced by the rolling process significantly affects the mechanical properties of rolled metals, and mechanical anisotropy caused by the rolling texture appears. Numerical reproduction of the rolling texture of the actual material reproduces the mechanical anisotropy of rolled metals in a crystal plasticity FE analysis.

This study investigates a method to reproduce mechanical anisotropy by accurately reflecting the rolling texture in an analytical model with a small number of grains for crystal plasticity FE analysis. We propose a method to extract the crystal orientation representative of the rolling texture from the crystal orientation measured by EBSD and reflect it in the analytical model. Using the presented method, we perform crystal plasticity FEM analysis. Based on the analysis results, the validity of the proposed model is discussed in comparison with conventional methods.

Room-temperature deformation behavior of semiconducting crystals

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Key Words: *Dislocations, Plastic deformation, Photomechanical effects, Photoindentation*

Generally, non-metallic compounds called ceramics and semiconductors are known to be brittle. This is partly due to the high Peierls potential, which cause higher force required for the motion of the dislocations responsible for plastic deformation. Recently, it has been reported that such materials can exhibit large plasticity even at room temperature by controlling the internal microstructure and/or outside external field. For example, we reported that quick room temperature deformation can be realized in strontium titanate ($SrTiO_3$) by using the internal elemental ratio close to the stoichiometric composition [1]. Also, we demonstrate a reversal of yield stress for $SrTiO_3$ crystals with different point defect concentrations and existing dislocation densities [2]. On the other hand, it was found that extraordinarily large plasticity appears in bulk compression of single-crystal ZnS in complete darkness even at room-temperature [3]. This is believed to be due to the less interactions between dislocations and photo-excited electrons and/or holes. However, methods for evaluating dislocation behavior in such materials with small dimensions under a particular light condition had not been well established. Therefore, we proposed a new nanoindentation method that incorporates well designed lighting system for exploring dislocation behavior depending on the light conditions in advanced semiconductors [4]. Then, we also used ZnS as a model material because its bulk deformation behavior has been well investigated. It is confirmed that the decrease of dislocation mobility with light observed in conventional bulk deformation tests can be understood even by the nanoindentation tests at room-temperature. It is remarkable that dislocation mobility appears to be more sensitive to light exposure than dislocation nucleation. Thus, we have investigated methods to plastically deform brittle materials and the effects of the internal microstructure and/or outside external field condition on the dislocation behavior. It is also attractive that the deformed brittle materials have a potential to exhibit unusual functional properties due to the special electronic states at around the dislocations cores [5-6].

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Spherulite Microstructure Formation Simulation Based on Effect of Molding Conditions on Polylactic Acid

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Key Words: *Crystalline polymers, Polylactic Acid, Spherulite, Mechanical Properties, Monte Carlo Simulation*

Thermoplastic polymers are increasingly being used in a wide range of fields because of their light weight, low cost and excellent formability. Crystalline polymers, which means thermoplastic polymers with semicrystalline phase, have a mixture of a crystalline phase with a stable folding structure of molecular chains and an amorphous phase with a disordered structure on a microscopic scale. These two layers are alternately stacked to form a structure: lamellar crystal. In addition, it is known that lamellar crystals grow radially to produce a crystalline structure, which is called a spherulite. The mechanical properties of crystalline polymers are closely related to the dimensions of the spherulite and the crystallinity, and the morphology of spherulite depends on the molding conditions such as temperature and pressure.

Evaluation of the effect of the spherulite microstructure on the mechanical properties of crystalline polymers can improve the accuracy of structural analysis. Various studies have been conducted on microstructure and crystallization models. However, since the spherulite is a complicated structure composed of amorphous and crystalline phases, the effects of actual molding conditions on spherulite microstructure formation and changes in mechanical properties depending on spherulite microstructure remain to be clarified.

This study investigates a simulation model predicting spherulite microstructure formation based on experimental observations. The crystallization process of polylactic acid is observed at different molding temperatures by in-situ observation, and the rate of spherulite formation and growth is estimated. Furthermore, according to the Turnbull-Fisher primary nucleation model and the Lauritzen-Hoffman secondary nucleation model, Monte Carlo simulations of spherulite microstructure formation are performed based on the obtained experimental results. The validity of the method is verified by a comparison of the simulated and the experimental results.

Study of Kink Strengthening of Polymer Materials with Mille-feuille Structure Based on FTMP Extended to Finsler Space

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Key Words: *Field Theory, Mille-feuille Structure, Polymer Material, Kink Strengthening, Crystal Plasticity*

FTMP framework has been extended to that in Finsler space, allowing it to additionally accommodate vectorial fields to be interpreted as "network microscopic degrees of freedom" representing "free volume" for modeling amorphous polymers. By utilizing thus extended FTMP, we perform here a systematic series of parametric studies of mille-feuille structured polymeric materials with different shear strength levels to investigate the conditions for the hard layers to yield "kinking" or fold buckling. Transverse stretching are subsequently carried out to further examine whether or not thus developed kinked mille-feuille structures can contribute to the additional strengthening. Demonstrated is the positive contribution to the stress rise, provided moderately kinked layers are formed during the pre-tension process, whereas over-stretched case tends to yield sudden stress drop accompanied by accelerated strain energy release, confirmed visually on the corresponding duality diagram, as well as physically via damaged region appeared on the corresponding strain energy fluctuation contour. For further examining the distinction between the two conditions, we performed extended simulatoins focussing exclusively on the MFS areas with and without a surrounding thin layer. A severely damaged region emerges in the late stage of transverse stretching for the overstretched model w/o thin layer, manifested as sudden volumetric strain burst, affecting also the free volume distribution, bringing about steep incompatibility rise on the duality diagram, whereas thin-layered model is shown to greatly mitigate the trend. This implies that the damage produced in the MFS region has been converted to the matrix in the full model, bringing about eventual stress drop.

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Systematic Inference of Interfacial Properties of Pure Materials by Phase-field Data Assimilation using Molecular Dynamics Solidification Simulation Results

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Key Words: *Data Assimilation, Phase-field Method, Molecular Dynamics Method, Interfacial Property Inference, Solidification*

Dendrites are a typical growing morphology for determining solidification microstructures. The phase-field method is the most accurate numerical model for expressing dendrite growth. However, there are serious issues in phase-field simulations of dendrite growth, such as the lack of solid–liquid interfacial properties of interfacial energy, interfacial mobility, and those anisotropy. Nevertheless, a conclusive prediction method of the interfacial properties has not been developed yet.

Recently, Ohno et al. [1] developed an inference method of the interfacial properties using data assimilation and phase-field method based on temporal change of solidification microstructures obtained by molecular dynamics simulation. This method can predict multiple interfacial properties simultaneously without setting special computational conditions. Nagatsuma et al. [2] also inferred the interfacial properties of a pure Ni through data assimilation.

In this study, we systematically infer the temperature-dependent interfacial properties of some pure metals through data assimilation. The temporal changes of solidification microstructures, which are used as the observation data, are obtained by molecular dynamics simulations using LAMMPS. Data assimilation is conducted based on the ensemble Kalman filter. To accelerate data assimilation with a massive number of phase-field simulations, we conduct parallel computations using multiple graphics processing units.

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Understanding power-law distribution in nanoindentation pop-in magnitude based on molecular dynamics simulation

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Key Words: *Plasticity, Nanoindentation, Pop-in, Power law, Molecular dynamics simulation*

Power laws are omnipresent and actively studied in many scientific fields, including microscale plasticity of materials. Recently, it was found that the magnitude distribution of second and subsequent pop-ins during load-controlled nanoindentation testing for body-centered cubic (BCC) iron (Fe) and face-centered cubic (FCC) copper (Cu) at room temperature obeys a power law in our previous study [1], and the obtained scaling exponent values were ≥ 3.0 and experimentally described to be much higher than those typically observed in micro-pillar plasticity, which are less than 2.0 [2][3]. Although the tendency of the exponents is partly suggested also in nanoindentation molecular dynamics (MD) simulations, systematic simulations, which are done in different temperatures and materials, have not been conducted yet. Further, although we suggested a theory of power law distribution for the pop-in size [1], the validity is still unknown.

In this study, we conduct a statistical analysis of pop-in magnitude in nanoindentation MD simulations for BCC Fe at 5, 300, 500, and 700 K and FCC Cu at 5 K. The obtained distributions of second and subsequent pop-in magnitudes follow power-law distributions. The values of scaling exponents are more than 3.0 for all the cases and decrease with temperature increases for BCC Fe cases. The results agree with the nanoindentation experiments and the suggested theory [1]. Furthermore, we discuss the validity of the theory by estimating the activation volume of dislocation migration from the equation in the theory and the simulation results. Including the previous study, we believe that the power law distribution seen in the nanoindentation pop-in magnitude provides a new insight into micro- and nanoscale plasticity in materials.

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Approximating Viscous Relaxation in a Hyperelastic Spherical Shell Subjected to Spherically Symmetric Deformation with Application to Modeling Foamed Rubber

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Key Words: *Rubber, foam, nonlinear viscoelasticity, model*

In order to better represent the volumetric time-dependent of foamed rubber, we examine the spherically symmetric response of a spherical shell comprised of an incompressible, hyperelastic material. The material is considered to be represented by a Parallel Rheological Framework as described by Hurtado *et al*. [1] with two networks which each have a Neo-Hookean elastic response. One of the networks has a power law viscoplastic response as well, allowing an elastic-plastic decomposition of the deformation gradient. We develop a solution algorithm to update the elastic Cauchy-Green tensors in the elasto-viscoplastic network at any given radial location based on the previous values at the point and a radial deformation applied on the outer surface of the sphere.

A numerical integration scheme is then demonstrated to update the total radial stress on the outer surface of the sphere approximately based on the internal stresses and radii at appropriate radial quadrature points. This approach is then used to describe the volumetric time-dependent response in a mechanical constitutive model for foamed rubber as an extension to the CHIPFoam model by Lewis [2]. Note that this model is appropriate for materials with moderate to high relative densities (0.3-0.99).

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Influence of the Pore Structural Parameters of Thermal Barrier Coating on its Modulus and Thermal Insulation

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Key Words: *Thermal barrier coating, Modulus, Thermal insulation, Microstructure reconstruction method, Pore structural parameters*

Thermal barrier coating (TBC) is one of the key thermal protection system for high-temperature components in gas turbines and aeroengines. Modulus and thermal insulation are two vital parameters that affect the performance and durability of the TBC system, which are close relative to the pore structural parameters (porosity, pore size, pore distribution, etc.) and has gained a lot of attentions in recent ten years [1]. While, to date, the influence of TBC's pore structural parameters on its performance is mainly theoretically investigated with ideal homogeneous pore model, or using local-image-based finite-element analysis method. These researches are not sufficient to statistically catch the real TBC's microstructure characteristics and reveal the specific performance of TBC with diverse pore structural parameters. Thus, in this work, a real-pore-microstructure-reconstruction method [2] is adopted to build the TBC's microstructure models with different porosities, pore sizes and pore distributions. Then the finite element method is used to study the variation of Young's modulus and thermal conductivity with pore structural parameters. It is found that [3], the microstructure with larger porosity and smaller pore size makes TBC the lower thermal conductivity, lower Young's modulus, providing better thermal insulation and thermal mismatch resistence for TBC system. In addition, the microstructure with smaller pore angle and larger pore aspect ratio has the lower thermal conductivity, and the microstructure with larger pore angle and larger pore aspect ratio has the lower Young's modulus. The above results may provide better understanding of TBC's failure mechanism, and have certain guiding significance for its future design.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Mesoscale Modeling of Carbon-Carbon Composite Manufacturing

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Key Words: Carbon-Carbon Composites, Manufacturing, Mechanical Properties, Thermal properties, Chemical Properties, Finite Element Analysis (FEA)

Spacecraft experience extreme thermal, mechanical, and chemical environments during atmospheric reentry. Some vehicles use a woven carbon-carbon (C/C) composite as a heat shield, where the carbon matrix is typically derived from pyrolized phenolic resins [1]. These composites are commonly used due to their exceptional material properties within these environments to protect and ensure survivability of the vehicle interior. However, designing new C/C based components for a wide variety of applications and atmospheric conditions is challenging. Fundamental knowledge of material properties across various length scales must be known. Additionally, understanding how manufacturing ultimately dictates performance must be well characterized.

To address the above challenges, we developed a mesoscale (tow-length scale) model of an idealized C/C composite geometry that simulates the manufacturing process. The geometry consists of woven tows impregnated with and surrounded by a resin, where the resin is modeled as a porous material. Decomposition of the resin is based on the Arrhenius equation, while pressure from pyrolysis gas formation are governed by Darcy's law and the ideal gas law for gases within open and closed pores, respectively. Mesoscale material properties are approximated using measurements of individual constituents, effective medium theory [2], and the Biot coefficient for porous solids [3].

A parametric study was performed to investigate the relationship among model input parameters and local stress concentrations. Initial results show a large increase in internal stresses during heating due to gas phase pressurization and shrinkage of the phenolic resin. While internal stresses continued to increase during cooling, they were small comparatively. Increasing the heating ramp rate had a large effect on the resulting stress, while little change occurred from varying the ratio of open to closed porosity.

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Elasto-plastic evolution of single crystals driven by dislocation flow

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Key Words: Dislocations, Crystal plasticity, Topological defects.

A model for large-strain, geometrically nonlinear elasto-plastic dynamics in single crystals will be presented. The key feature of this model is that the plastic dynamics are entirely driven by the movement of dislocations, that is, 1-dimensional topological defects in the crystal lattice. It is well known that glide motion of dislocations is the dominant microscopic mechanism for plastic deformation in many crystalline materials, most notably in metals. However, a comprehensive model linking the dynamics of individual dislocations to elaso-plastic evolution has been missing to date.

A geometric language is proposed, built on the concepts of space-time "slip trajectories" and the "crystal scaffold" to describe the movement of (discrete) dislocations and to couple this movement to plastic flow. The energetics and dissipation relationships in our model are derived from first principles drawing on the theories of crystal modeling, elasticity, and thermodynamics. The resulting force balances involve a new configurational stress tensor describing the forces acting against slip. In order to place our model into context, it can be shown that several laws known in special cases before can be recovered, most notably the equation for the Peach–Koehler force (linearized configurational force) and the fact that the combination of all dislocations yields the curl of the plastic distortion field.

The mathematical framework developed has enabled existence proofs for some special cases of the model, and the development of new tools in geometric measure theory. Details of these are referenced below.

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Geometric modelling of dislocation motion

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Key Words: Dislocations, crystal plasticity, elasto-plastic evolution, topological defects

This talk presents a novel geometric language [1, 2] to describe the movement of dislocations, which is built on the concept of space-time *slip trajectories*, that is, the 2-dimensional surfaces "traced out" by the dislocations as time progresses. This in particular allows one to compute all relevant quantities (Burgers vector, slip velocity, dislocation orientation, etc.) in a straightforward way and thus to directly couple the dislocation dynamics to plastic flow. One decisive feature of this approach is that it retains more information than the corresponding Kröner dislocation density tensor (which can be computed from the geometric description, but not the other way round).

The geometric language can furthermore be made mathematically rigorous, furnishing a "weak formulation" of the equations describing dislocation motion. This then enables a proof [3] of the well-posedness of the associated rate-independent (quasi-static) system of large-strain elasto-plastic evolution driven by dislocation flow.

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Modeling Frictional Behavior in Rupture Dynamics using Field Dislocation Mechanics

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Key Words: Rupture Dynamics, Dislocation Mechanics, Static and Dynamic Friction, Short slip

We model important physical observations in rupture dynamics including static and dynamic friction, short-slip and slip obtained via crack-like models, using field dislocation mechanics (FDM). FDM is a non-linear pde based model of the mechanics of dislocations, where individual dislocation are treated as a continuously distributed field, instead of singular lines, and the plastic deformation is accounted for due to motion, interaction and nucleation of dislocations [1].

We utilize an ansatz to produce an exact, reduced, plane model of FDM, where the dislocations are allowed to move in a planar fault layer (which is sandwiched between elastic blocks), as initially developed by Zhang et. al (2015) [1]. The model yields a non-linear Hamilton-Jacobi (H-J) equation for the evolution of plastic shear strain enabling the representation of a propagating rupture front. The plastic strain in the fault layer is assumed to damage the elastic modulus behind the rupture front. This leads to an energetic driving force contribution for evolution of plastic strain that was noted, but not accounted for, in the rupture-related simulations in [1]. Here, we account for this driving force to complete the self consistent evaluation of the rupture model. The H-J equation for front propagation is solved using an implementation of a *Central-Upwind* scheme developed by Kurganov et. al (2001) [2].

Our simulations recover static and dynamic friction laws as emergent features of our continuum model, also resembling the Mohr–Coulomb failure criterion for geomaterials, including well-defined features of cohesion and friction angle. As in earlier work [1], we are also able to recover the short-slip with lesser 'elastic damage' behind the front, as well as the square-root dependence of slip on time for the greater damage (crack like model) case with the present algorithm.

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Strain-induced Change of Adsorption Behaviour of Gas Molecules on Graphene: A first-principles Study

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Key Words: *First Principles Calculation, Adsorption of Gas Molecules, Graphene, Strain, Electrical Resistance,*

Graphene has been suggested to be capable of detecting gas compositions in a person's breath to diagnose sickness down to the ppb-level [1,2], because of its large surface-to-volume ratio and high carrier concentration. The resistance of graphene was found to change clearly due to the adsorption of gas molecules such as CO, NO_2, and so on. When plural different molecules adsorb on graphene at the same time, however, it is impossible to identify the adsorbed molecules individually. The development of the selectivity of the adsorbed molecules, therefore, is indispensable for applying this gas-adsorption-induced resistance change of graphene to a health monitoring sensor. Since the mixed gas in a person's breath is a natural environment, understanding how to detect a target object selectively is of permanent interest to the development of novel gas sensors. Recently, it was found that the effective activation energy of chemical reactions varies drastically under the application of mechanical stress and strain [3]. This result indicates that the adhesion energy of gas molecules can be shifted from negative one to positive one under the application of appropriate strain.

In this study, the strain-induced change of adsorption behaviour of gas molecules on graphene was analyzed by using first-principles calculation to achieve selective detection of gas molecules. First, the optimal adsorption positions for each gas molecule (CO, H_2O, NH_3 and NO_2) on graphene were determined by using adsorption energy E_{ad} and Bader charge transfer ΔQ. Then, change of the E_{ad} and ΔQ was analyzed under the application of uniaxial strain to graphene from -10% to 10%. It was found that both values changed almost linearly with the applied strain. In addition, there was a critical strain of each molecule at which adsorption energy changed from negative value to positive value, in other words, adsorption behaviour changed to desorption behaviour. This result clearly indicated the possibility of the selectivity of gas molecules which adsorb on graphene by applying appropriate strain. The change of the current-voltage (I-V) relation of graphene under the adsorption of gas molecules was also analyzed using nonequilibrium green's function (NEGF) formalism. It was confirmed that the I-V curves altered obviously with the change of the adsorbed molecules and applied strain. These findings clearly showed that the adsorption behaviour on graphene can be tuned by external strain for multi-object detection, paving the path for graphene-based gas sensor in biosensing applications.

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Theoretical study on strain-controllable electron transport properties of dumbbell-shape graphene nanoribbon

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Key Words: *graphene nanoribbon, dumbbell-shape, strain-controlled, atomic seamless interface, first-principles*

Abstract:

When a graphene is cut into a narrow ribbon with nano-scale width, referred to as graphene nanoribbon (GNR), a GNR starts to show semiconductor properties. To employ a semiconducting GNR as the device element, a metal electrode must be attached to the GNR to form stable ohmic contact and conduct current through the GNR. In order to develop a simple and versatile method for forming ohmic contacts between metal electrodes and GNRs, we have proposed a novel structure named the dumbbell-shape GNRs (DS-GNRs) [1]. The dumbbell-shape structure consists of one narrow segment sandwiched by two wide segments. Since GNRs in the wide segments of the DS-GNR exhibit metallic electronic properties, ohmic contact with metal electrodes can be expected, and in fact, the I-V characteristics of a GNR with a width of 40 nm in the narrow segment have been successfully measured by applying the dumbbell-shape structure. On the other hand, since a DS-GNR comprises both metallic and semiconducting regions in one molecule (structure), Schottky barrier is expected to form at the junction interface between the wide and narrow segments. Therefore, the electron transport properties of DS-GNR is expected to be strongly affected by the electronic state of this junction interface. In this study, first-principles calculations based on density functional theory were performed to analyze in detail the electronic transport properties of DS-GNRs and the strain dependence of their current-voltage characteristics (I-V characteristics).

The electronic band structure of a dumbbell-shape structure consisting of a semiconducting GNR with a band gap of 1.6 eV in the narrow segment and GNRs with metallic conduction properties in the wide segments was investigated. In the longitudinal direction of the narrow segment from the junction interface betwen wide and narrow segments, the region was divided into units with the length of a six-membered ring of carbon atoms as one unit, and the density of states analysis was performed for each region. The energy barrier for electronic conduction between each region was defined by the energy difference of the lowest conduction band in each region. A clear energy difference of conduction band was observed between the junction interfaces between the wide and narrow segments, indicating the existence of a large energy barrier (Schottky barrier) near the junction interface. In the narrow segment near the junction interface, new electronic states appeared within the 1.6 eV wide forbidden band due to the exudation of a wave function from the wide segment into the narrow segment. As a result, the energy barrier in the narrow segment was not constant, but a gradient Schottky barrier appeared, in which the minimum energy of the conduction band increased monotonically from the junction interface region to the central region of the narrow segment. Furthermore, the gradient Schottky barrier changed as the band gap of the narrow segment decreased due to uniaxial tensile strain, and it was confirmed that the Schottky barrier disappeared at 8% tensile strain, and the junction interface between the wide and narrow segments became a metallic-metallic junction. Therefore, it is feasible to control the gradient Schottky barrier and switch from semiconducting to metallic conduction in the dumbbell-shape GNR by applying an appropriate range of strain.

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Experimental analysis and numerical modeling utilizing fractional calculus of selected roofing felts

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Key Words: roofing felt, mechanical material anisotropy, microstructure of roofing felts, chemical composition of roofing felts, scalar damage; fractional calculus; damage mechanics

Due to its low cost and relatively simple installation, roofing felt is well-known material for decades and is still widely used as a waterproof insulation in commercial and residential buildings. They are available in many types and variants, differ in purpose, thickness, materials or finishing.

In presentation, we will focus on a selected representatives of this group. Research methodology, results of determination of detailed mechanical behaviour, microscopic photos of the material structure and maps of chemical composition of different types of roofing felt will be presented. The presented results will show how heterogeneous and anisotropic structure the roofing felt is.

Based on the obtained results computational modelling strategy utilizing hyperelastic fractional damage material model with memory presented by W. Sumelka and G.Z. Voyiadjis in [1] will be presented. Results of numerical analysis have been prepared with symbolic mathematical calculations software *Wolfram Mathematica* extended with *AceGen/AceFem* software in which implementation of the concept of hyperelastic fractional damage material model with memory has been prepared. The choice of *AceFem* software was dictated by its structure (the system combines symbolic and numeric approaches) and because its environment is designed to solve multi-physics and multi-field problems.

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Model-order reduction of locally resonant metamaterial plates

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Key Words: Model-order reduction, Modal analysis, Dynamic-stiffness method, Local resonance

A reduced-order dynamic-stiffness method is formulated in order to compute the dynamical response of locally resonant metamaterial plates, i.e. plates coupled with periodical arrays of resonant subsystems. The formulation rests on a dynamic-stiffness model obtained by exact condensation of all the degrees of freedom within the resonators. The main results are twofold: a) after having built the global dynamic-stiffness matrix, the natural frequencies and undamped modes are computed by means of the Wittrick-Williams algorithm [1, 2, 3]; b) two orthogonality conditions are derived for the modes associated to the plates only and employed to find closed analytical forms for the modal response under arbitrary loads, both in time and frequency domain, under the assumption of classical damping [4, 5]. The results are compared with finite-element solutions assessing the accuracy of the proposed formulation.

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Numerical analysis of Portevin-Le Chatelier effect using regularized large strain thermo-visco-plastic model

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Key Words: PLC effect, large strain thermo-visco-plasticity, regularized Estrin-McCormick model

The research presented in this paper is focused on the numerical simulation of a propagative instability called Portevin-Le Chatelier (PLC) effect using large strain thermo-plasticity models. The PLC effect is attributed to dynamic strain aging and characterized by serrated response (stress-jumps) in the stress-strain plot, related to moving shear bands. It affects several material parameters like the yield stress, hardening rate (and thus material ductility) and ultimate tensile strength. The PLC effect occurs in metals, for example steel and aluminium alloys, under certain strain rate and temperature conditions [1].

A large strain thermo-visco-plastic Estrin-McCormick model [2] is employed in the analysis. The McCormick part of the model is based on [3]. The thermo-visco-plasticity formulation is an extension of the work [4]. It incorporates strain hardening, strain rate sensitivity to represent viscosity as well as the dynamic strain aging, and thermal softening. The rate-dependence is treated in the model as a regularization method, but the model is also optionally equipped with a gradient enhancement.

A parametric study for different values of strain rate, temperature, strain ageing time and, when relevant, internal length is carried out. Comparisons with experimental data from [5] are performed. All computations are executed using AceFEM and AceGen numerical packages within Wolfram Mathematica [6]. Viscosity is shown to be necessary to avoid problems with convergence. Moreover, the influence of the gradient enhancement on the simulations is evaluated. Good agreement with experimental findings in terms of global load-deformation response is obtained, but a model correction is needed to eliminate serrations in the post-peak (necking) regime.

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Plastic Hinge Formation in the Framework of the Space-Fractional Beam Theory

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Key Words: non-local models, plastic hinges, elastic-plastic bending, fractional calculus

The study presents recent results on nano/micro-beam modelling in the framework of space-Fractional Continuum Mechanics. According to this formulation, the scale effect is modelled using fractional derivatives and determined by parameters: α (order of fractional derivative) and ℓ_f (length scale).

The development of space-Fractional Euler-Bernoulli and Timoshenko beams theories considering elastic-plastic properties will be presented. The Huber-Mises-Henky plasticity criterion, isotropic hardening, and grain-size-dependent strengthening (described by the Hall-Petch relation) will be included. A significant result is a demonstration that the material microstructure determines the scale effect. In particular, it will be identified that the length scale ℓ_f is represented by the grain size of a microstructure. The presentation will include the effect of microstructure on the formation of plastic hinges for beams under bending.

In conclusion, consideration of the microstructure is essential in analyzing nano/micro-beams, and a direct reference to the microstructure is possible with fractional models.

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Integrated Method of Inverse Isogeometric Analysis and Distributed Fiber Optic Strain for Monitoring Structure Deformation and Stress

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Key Words: *Inverse-Isogeometric Analysis, Distributed Fiber Optic Sensing, structural monitoring, strain, stress*

Remote monitoring of structures is an important advance in modern engineering for safety, maintenance and management purposes. Recent developments in sensor technologies, fast data communication networks and Internet-of-Things enabled the prospect of smart structures which can be observed remotely for real-time changes in deformation and stress distribution.
Distributed Fiber Optic Sensing (DFOS) is an excellent sensor of choice for structural monitoring applications because of its light weight, high spatial resolution, high accuracy and resistance to harsh environments [1]. However, measured fiber strain data from DFOS must be translated to structural deformation and stress using a numerical inverse analysis method. Isogeometric Analysis (IGA) is a good candidate for this purpose since its higher efficiency and accuracy over traditional FEM has been proven [2, 3, 4].
In this work, an integrated method of inverse IGA and DFOS fiber model is proposed. This method can be used to calculate the deformation and stress distribution of a structure from measured fiber strains. In the proposed method, both structure geometry and fiber geometry are modelled using Non-Uniform Rational B-Splines (NURBS) functions which constitute the core of IGA. This integrated approach not only enables direct input from Computer-Aided Design (CAD) models for streamlined practical application but also improves the efficiency of numerical calculations. In addition, spatial resolution and sampling locations can be changed to match the measurement mode of DFOS instrument which is not possible in fixed point-sensor models.
The proposed method is first verified with a simulated example. Then, it is applied to a practical model using measured DFOS data from experiment. The results show that the inverse method is accurate, fast, robust and can accurately reproduce structure deformation and stress using the measured strain distribution in the optical fiber direction. Hence, the method shows a promising potential for industrial applications.

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Ultrasonic Testing and Imaging of Out-of-plane Fiber Wrinkling in Multilayer Composites with Double-side Pulse-echo Methods

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Key Words: *Composites, Ultrasonic testing, Layered structure, Out-of-plane wrinkling, Imaging*

Abstract. Fiber reinforced polymers (FRPs) have been increasingly used in various fields. However, fiber wrinkling in manufacturing and service will have a great impact on the mechanical properties of composites, which requires non-destructive testing and evaluation (NDT&E) for potential structure defects[1]. Considering that a purely analytical approach relied on the assumption of plane wave, e.g. recursive stiffness matrix[2], fails to offer accurate ultrasonic Ascan signal for wavy FRP, this study builds dedicated FRP models with out-of-plane fiber winkling using the cloud-based commercial finite element simulation platform OnScale[3], in order to assess the fiber wrinkling in the layered FRP. Then the wrinkling imaging is performed in the ultrasonic Bscan imaging by information extraction from the echoed signals based on the principle of interply resonance, in which several parameters, including signal amplitude, phase, frequency, and bandwidth, are studied for improvement of imaging quality. The analysis result indicates that the single-side pulse-echo method may give false waviness imaging results at local regions attributed to the wave beam deviation from the fiber wrinkling. Hence, a double-side ultrasonic testing method is proposed, i.e. to excite ultrasound from both sides of FRP, in order to optimize the out-of-plane fiber wrinkling imaging quality. In the proposed method, two imaging results from each single-side pulse-echo are superposed with different weights at each specific imaging region, thereby improving the imaging effect. The proposed method has great potential on FRP characterization of fiber wrinkling in the manufacturing stage.

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Variational Mode Decomposition of the Contact Ultrasonic Testing Results for Wood Quality Assessment

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Key Words: Contact ultrasonics, Variational Mode Decomposition, Feature engineering, Instantaneous frequency, Statistical features

The contact Ultrasonic Testing (UT) technique has been widely used for Non-destructive Damage Testing of different materials such as wood. In this light, the time of flight and velocity of the ultrasonic wave in a wood section has been traditionally monitored and correlated with the wood quality. However, the results of such practice have not been satisfactory, prompting researchers to devise new strategies to tackle the problem. This study mainly focuses on the feature engineering of contact ultrasonic testing results for the quality evaluation of wooden sections. To this end, the Variational Mode Decomposition algorithm is employed to extract some informative features out of ultrasonic signals to be fed into Machine Learning (ML) algorithms. The developed ML algorithms are set to solve some supervised classification problems based on data gathered from testing specimens with different health conditions. Artificial hole defects, of various sizes, have been introduced to the specimens to simulate different severity of the defect in the specimens. The study focuses mainly on the effectiveness of different types of features in solving the classification problem of wooden specimens based on their health state. To this end, different features are obtained out of the extracted modes of the ultrasonic testing result, including the centre frequency of the extracted modes, the root mean square value of the instantaneous frequency of the modes, as well as some statistical features such as mean, median, skewness and kurtosis of the instantaneous frequency of the modes. A comprehensive comparison of the obtained classification results is made when different types of features were fed into the classification problem.

Varying-pitch comb-shape DW sensor for UGW based SHM

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Key Words: *Ultrasonic Guided Wave (UGW), Direct-Write (DW) Sensor, Comb-Shape, Wave Mode Match/Mismatch*

The low profile, lightweight and flexibility of direct-write (DW) sensors made of piezoelectric coatings have great advantages in ultrasonic structural health monitoring (SHM) applications. The DW sensors can be printed on the surface of the structure or embedded into the structure through scalable processing with improved consistency and lowered implementation cost. To selectively excite and receive the ultrasonic guided wave (UGW) signal, a comb-shape DW sensor is usually designed with element pitch same as the mode wavelength. A good match between the element's pitch and the wavelength of the designed mode is crucial for accurately and efficiently recording the arrival signal. In real situations, the structural and material properties may not be uniform or degraded during in service. Changes in these properties may alter the UGW wavelength, causing a deviation in the match between the comb-shape sensor and the pre-selected wave mode. As a consequence, the designed comb-shape sensor may fail due to an inaccurate evaluation of wave received.

In this paper, we first examine the effect of mismatch of comb-shape sensors on the wave arrival time in an adhesive structure (Al-Epoxy-Al). To simulate the mismatch phenomenon, the degradation of adhesive material properties and the variation of adhesive thickness in actual adhesive structures are taken into account when modeling the adhesive layer. By selecting an appropriate UGW mode, it can be determined whether disbond has occurred in the adhesive layer based on the differential arrival time of the wave. However, the wave arrival time in the disbond case may be completely different from the design stage when the mismatch occurs. This mismatch prevents the comb-sensor from detecting disbonds in adhesive structures. To solve this challenging mismatch problem, we present a new comb sensor design that can adapt to the mode wavelength. In the new design, the pitch and width of the elements can vary with the length of the elements. Pitch variations are tuned to correspond the changes in mode wavelength. Simulation results showed that the high-amplitude wave packet can correlate to the designed mode packet. Accordingly, the varying-pitch comb-shaped sensor provides a more reliable evaluation of structural health by adapting to the mode wavelength.

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Anomalous diffusion: Fractional models and application

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Key Words: *Anomalous diffusion, Fractional derivative, Complex media, Non-locality*

Heterogeneity embedded in natural media and flow field challenge the application of Fick's 1st Law in anomalous diffusion well documented in many disciplines. Anomalous diffusion is one of the major topics in theoretical physics and statistical mechanics, and it is also the fundamental physical process with good potential application in environmental and hydrologic sciences and engineering. As a novel modeling tool in mathematics and physics, the fractional-order derivative diffusion equation models characterize anomalous diffusion with history-dependence and spatial non-locality, accurately describe the tailing in breakthrough curves of solute transport. We summarize the recent progresses and discuss the key challenges of fractional derivative diffusion equation models including the existed research and current development, fractional derivative modeling, numerical algorithms, and related applications in the field of environmental fluid mechanics. Here also made some preliminary discussions on issues of fractional derivative diffusion equation model, such as statistical description, model parameter determination and dimensional analysis, which may contribute to the further study of anomalous diffusion.

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Domain Decomposition Solvers for Nonlocal Equations

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Key Words: Nonlocal equations, domain decomposition, FETI

We present a domain decomposition method for the efficient simulation of nonlocal problems. Our approach is based on a multi-domain formulation of a nonlocal diffusion problem where the subdomains share "nonlocal' interfaces of the size of the nonlocal horizon. This system of nonlocal equations is first rewritten in terms of minimization of a nonlocal energy, then discretized with a meshfree approximation and finally solved via a Lagrange multiplier approach in a way that resembles the finite element tearing and interconnect method. Specifically, we propose a distributed projected gradient algorithm for the solution of the Lagrange multiplier system, whose unknowns determine the nonlocal interface conditions between subdomains. Several two-dimensional numerical tests on problems as large as 191 million unknowns illustrate the strong and weak scalability of our algorithm, which outperforms the standard approach to the distributed numerical solution of the problem. This work is the first rigorous numerical study in a two-dimensional multi-domain setting for nonlocal operators with finite horizon and, as such, it is a fundamental step towards increasing the use of nonlocal models in large scale simulations.

Extended Bond-based Peridynamics with Plasticity

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Key Words: *Bond-based peridynamics, Plasticity, FEM/XPDM coupling, Numerical modelling, Quasi brittle materials*

Cohesive-frictional materials usually experience inelastic deformations during their progressive damage. In constitutive modeling, the classical peridynamic theory has gained increasing interests in describing elastic damage and failure of brittle materials essentially by means of bond breakage. In order to remove the limitation of the Poisson's ratio, the bond-based peridynamics has been recently enriched with bond rotation effects.

In order to enlarge its application particularly for geomaterials which presents material damage and inelastic deformation under compressive loading, the present paper aims at integrating the description of plastic strains into the extended bond-based peridynamic model (XPDM). For that, the total strain approximated locally is decomposed into an elastic part and a plastic part. The evolution of plastic strains is determined in the classical plasticity theory. In other words, commonly used elastoplastic models can be incorporated directly in the proposed framework.

For validation, the von Mises type yield function without hardening effect and the Drucker-Prager type yield function with an isotropic plastic hardening are taken into account for validation purpose. On numerical aspects, the XPDM with plasticity is implemented by following a peridynamic/finite element coupling procedure. Numerical predictions by the XPDM with plasticity are compared with those from finite element analyses and experimental data. In that process, numerical accuracy and computational efficiency of the proposed method are assessed.

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Fatigue crack propagation simulated by using a FEM-peridynamics coupled method

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Key Words: *peridynamics, fatigue crack propagation, non-local methods*

Fatigue crack propagation in structural materials is one of the most common problems in aeronautical applications where cracks are closely monitored on the field with very limited attempts to simulate their evolution. In this study Peridynamics (PD) [1,2] a nonlocal continuum theory formulated with integral equations, is adopted to simulate the crack propagation due to fatigue phenomena. Inspired by [3] the peridynamic formulation has been enriched introducing a damaging effect due to the high cycle fatigue phenomena applied to a bilinear constitutive law [4]. Consequently, the fatigue degradation of the bond stiffness can be evaluated. The total load is composed by blocks of cycles, each block is characterized by a fixed load amplitude and a given number of cycles. Two components of damage increment are considered: the static damage, and the fatigue damage, both of which contribute to defining the damage state of the material.
Furthermore, combining the capability of Peridynamics in modelling crack propagation with a FEM-PD coupled method [5] the computational effort can be reduced. Peridynamics is adopted in the region of the model where the crack is expected to propagate while the remaining part of the specimen is discretized by using FEM.
The proposed approach is applied to model 2D structures in presence of voids and inclusions under fatigue load conditions considering isotropic homogeneous and heterogenous materials. Results are evaluated taking into account different mesh sizes, horizon dimensions, crack initial lengths and crack orientations to demonstrate the capabilities of the proposed method.

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Fully anisotropic peridynamics with pair-potentials

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Key Words: Peridynamics, Multiphysics Problems, Anisotropy, Fracture

We present an in-plane anisotropic continuum-molecular formulation for elasticity, fracture and diffusion-based problems in the peridynamic theoretical framework. Following a mechanistic approach, we define constitutive laws for long-range interactions such that the macroscopic behavior of the material is the result of the assigned micro-interactions properties. Elastic and inelastic pair potentials act on interacting oriented material points within a cutoff distance and enable to derive pairwise actions as energetic conjugates to specific pairwise deformation measures. The non-central force assumption, together with the definition of specific direction-dependent micro-moduli functions respecting material symmetries, allow to obtain a continuum formulation for anisotropic media using a purely pairwise descriptions of deformation and general constitutive properties. Non-uniform material toughness is modeled adopting an anisotropic energetic failure criterion related to direction-dependent fracture energy functionals. This is the first two-dimensional fully anisotropic bond-based type model without restrictions affecting the number of independent material moduli. Applications proposed include comparison against analytical solutions and fracture and damage sensing in conductive tissues.

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Investigation of wave propagation of a one-dimensional bi-material system

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Key Words: *Nonlocal problems, Bi-material system, Conservation laws, Wave reflection*

ABSTRACT:

In this talk, we explore the theory and implementation of wave propagation in a one-dimensional bi-material system using the local and nonlocal models, respectively. The local description is based on a coupling of two local continuum mechanics and the nonlocal description is based on a coupling of two nonlocal peridynamics with different constants. To study the physical reflection coefficients and diminish the artificial reflection rising from the simulation, one need to maintain the conservation laws across the material interface on a discrete level. We study the conservation laws of linear momentum and total energy for both local and nonlocal models in a continuous setting and then propose the numerical discretization accordingly to preserve those quantities. We test various propagating waves to study the reflection coefficients in a one-dimensional bi-material system. Several numerical tests are performed to confirm our theoretical findings.

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Meshfree methods for fractional PDEs using Gaussian kernels

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Key Words: Radial basis functions, meshfree methods, fractional PDEs, nonlocal models

There has been a growing interest in the study of nonlocal models and fractional PDEs as more general and sometimes more realistic alternatives to the conventional PDE models. However, high computational cost could be induced by numerical approximations of integral formulations of nonlocal derivatives. Meshfree methods based on radial basis functions (RBF) provides an alternative to solve fractional PDEs without the use of numerical quadratures. Although computationally convenient, there is little understanding of the properties of meshfree methods for fractional PDEs based on RBF. For example, stability of the numerical methods is not guaranteed theoretically and the way to choose the RBF shape parameter is ad-hoc. In this talk, we will introduce a stable RBF meshfree method for fractional PDEs using Gaussian kernels where the RBF shape parameter is correlated with the mesh parameter. We study the convergence of the proposed method and provide numerical examples for practical guidance.

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Peridynamic Modeling of the Dynamic Failure of Additively Manufactured Steel

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Key Words: *Additive manufacturing, spall, shockwave, peridynamic, crystal plasticity, impact*

Because nonlocal methods do not assume or require continuous displacement fields, they allow a computational model to capture the nucleation and progression of damage with potentially great generality. In this work, the effect of microstructure on the high-rate tensile failure (spall) of additively manufactured 304L stainless steel is studied. The simulation method uses state-based peridynamics with a new model for the time dependence of high-rate failure within grains. A crystal plasticity model incorporates anisotropy in the elastic and plastic response of the grains. The grain shapes and lattice orientations are initialized directly from Electron Backscatter Diffraction (EBSD) images.

The model results are compared with test data from plate impact experiments over a range of impact velocities. Although it takes place within a very short time interval, the process of dynamic failure has an observable effect in the measured data. This effect is, to a large extent, reproduced by the model.

Simulations with different realizations of the microstructure reveal the sensitivity of the failure process to the random nature of the grains. This is important with additively manufactured steel because of the wide variations in sizes and shapes of grains at different positions within the sample.

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Peridynamics Computations at the Exascale

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Key Words: *Peridynamics, Large-Scale Fracture Simulations, GPUs, Performance Portability, Exascale Computing*

Peridynamics is a nonlocal reformulation of classical continuum mechanics suitable for material failure and damage simulation, which has been successfully demonstrated as an effective tool for the simulation of complex fracture phenomena in many applications. However, the nonlocal nature of peridynamics makes it highly computationally expensive, compared to classical continuum mechanics, which often hinders large-scale fracture simulations. In this talk, we will present ongoing efforts to develop a GPU-enabled, performance portable, and exascale-capable peridynamics code designed to run on U.S. Department of Energy supercomputers, in particular Summit (currently ranked #2 in the TOP500 list) and Frontier (to be deployed later this year), both at Oak Ridge National Laboratory.

Combined finite-discrete element simulations for multi-body dynamics and fracture mechanics

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Key Words: *FEM, DEM, FDEM, Fragmentation, Multi-body Systems, Industrial Processes*

The key features of the combined finite-discrete element method (FDEM) [1] are the following: (a) compute the contact interaction and motion of bodies, (b) calculate the stresses and deformations and (c) compute the transition from continua to discontinua when fragmentation occurs.
This talk will cover some of the most recent applications of FDEM for multi-body dynamics and fracture mechanics. This includes applications to the packing and breakage of catalyst pellets, fibre-reinforced concrete tunnels, armour units for coastal defence, and the simulation of breakouts and solid production in drilled rock formations [2, 3, 4, 5]. Some of the discussion will focus on open problems and on the challenging aspects of FDEM in fracture simulations, such as the joint-element induced artificial compliance, element size constraints due to the discretisation of the process zone, dynamic effects induced by the application of boundary conditions (e.g. in-situ stresses), and others.

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Creating Digital Twins for Human/Society and System/Service with Uncertainty and Complexity

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Key Words: *CPS, Digital Twin, Surrogate Model, Complex Network, SCM, Society5.0*

In VUCA (Volatility, Uncertainty, Complexity, Ambiguity) era such as COVID-19 pandemic, global manufacturing industry should be transformed into the new paradigm of smart manufacturing based on Cyber Physical Systems (CPS) with Digital Twins including uncertainty and complexity of human/society and systems/services. Especially concerning to the global supply chain management (SCM) network which is heavily damaged under COVID-19 pandemic, the complexity of the network structure should be considered and modeled properly for the inclusion to the Digital Twins.

In MS196 of WCCM2020, we have introduced the foundation of "Computational Information Science" in order to incorporate the human and the society into the Digital Twin models for the implementation of the smart services in Society5.0[1)]. On the uncertainty quantification of the CPS process, the human and the society have quite wide range of uncertainty for the modeling of human behavior and social decision making. We have defined Uncertainty of Things as the uncertainty in data from devices and uncertainty in Digital Twin models which are created as Surrogate Models from CAE analyses and Machine Learning regressions. Also, we have defined Uncertainty of Subject as the uncertainty of the human and the society, which are the beneficiaries receiving services and have bounded rationality of human based upon Prospect Theory[2)]. Then, we will introduce Digital Twin model for SCM process having complexity and fragility based upon Complex Network theory[3)].

Finally, Digital Twins for design process, production process, global SCM process and service delivery process are introduced and discussed in view of realizing human centered Society5.0. Furthermore, we will consider the crisis recognition of the global manufacturing industry and the global supply chain logistics from a new perspective, including uncertainty and complexity. In order to promote business transformation (DX) under new-normal condition, we will create Digital Twins with CPS including SCM and value chain networks.

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Digital Triplet for Recording and Reusing Engineering Processes Executed by Human Intelligence

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Key Words: *Digital Twin, Digital Triplet, Cyber Physical Production System*

The rapid digitalization is changing the manufacturing paradigm as Industrie4.0 exemplifies. Japanese manufacturing industry seems to be falling behind this digitalization. We should transplant the strength of Japanese manufacturing industry, if there is, to the new vessel (namely, digitalization). Perhaps the strength is high-quality in manufacturing, which results in high-quality products and cost down and no defect in production. For transplanting the strength of Japanese manufacturing industry or to a new vessel, we are proposing *Digital Triple*. Since Industrie4.0 takes rather a top-down approach, it is difficult to make full use of field experts' knowledge and skill, which are typical strongest points of Japanese manufacturing industry. For solving this issue, Digital Triplet aims to support engineers and technicians to solve problems and to crate various values throughout a product life cycle, which leads to human centered digital manufacturing.

While CPS or digital twin consists of physical world and cyber world, Digital Triplet consists of physical world, cyber world, and intelligent activity world done by human so as to create values from data and information by employing human knowledge. Digital Triplet integrates these three worlds to realize the integrated support of engineering activities throughout a product life cycle.

Specifically, we propose a novel method for structurally describing decision-making processes by mapping intention and judgment of engineers to actions on CPPS. Digital Triplet aims at recording various engineering processes executed by engineers on cyber physical systems and supporting other engineers by reusing the recorded engineering processes.

Finally, this study illustrates an experiment for performance improvement by engineers on the prototype system of a learning factory. The experiment verified that the Digital Triplet concept is successfully realized, and the proposed method is effective to represent the engineering processes of engineers.

Modelling Cognitive Bias in Safety using Bayesian Inference

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Key Words: *Safety, Perception, Cognitive Bias, Bayes, Covid-19*

In a human centred society, sense of safety perceived by people is important to consider as well as actual safety. The gap between expectations and reality in safety causes social problems. Overestimation of safety provokes dangerous behaviours, while underestimation of safety causes excessive behavioural restraint. For example, in COVID 19 pandemic, the overestimation may lead to the spread of infection due to dangerous behaviours, and the underestimation may lead to slow consumption due to excessive self-control.

In this talk, I propose a mathematical framework to model sense of safety using Bayesian inference. Recent neuroscience studies suggest that human brain activities can be explained as a Bayes' model(Knill & Pouget, 2004). Here, based on Helmholtz's epistemology, I assume that safety x is inferred as the cause of observation (data: y) and define the sense of safety as Bayesian posterior $p(x|y)$ that is proportional to a product of a prior $p(x)$ and likelihood $p(y|x)$. The prior and the likelihood represent the expectation of safety and the safety based solely on the data (observed safety), respectively. In this model, the prior (safety belief) is updated to the posterior (perception of safety).

The difference between the posterior mean and the peak of likelihood represents the gap between perceived and observed safety. This gap is regarded as a cognitive bias termed *expectation effect* (Yanagisawa, 2016). In our previous study, we modelled the expectation effect as a function of three parameters: a prediction error (difference between prior mean and peak of likelihood), prior precision (inverse variance of the prior), and observation precision (inverse variance of the likelihood). We found that there are two types: assimilation and contrast. Assimilation diminishes the prediction error, and contrast exaggerates the prediction error. The expectation effect explains several psychological biases that lead to abnormal behaviours, such as normalcy bias, excessive anxiety, and overconfidence. Based on the expectation effect model, I discuss the condition of each psychological bias in safety. In addition, I discuss how to model emotions such as anxious and fear in a mathematical manner by applying information theoretic quantities such as surprisal and free energy (Yanagisawa, Kawamata, & Ueda, 2019).

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Overview of the HEXAGON-TUS Joint Research: A Strategic Effort to Infiltrate Manufacturing Digital Twin Competency into Industry

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Key Words: *Digital Twin, Smart Manufacturing, High-Fidelity Simulation, IoT, Data Science*

Recently, there are more opportunities to hear the term Digital Twin (DT). In particular, it is often used as one of the elements to realize the "super-smart society" set forth in Society 5.0 described in the 6th Science and Technology Basic Plan (2021-2025). While DT used to be mainly discussed in the manufacturing context as for Industry 4.0, recent DT is extensively even focused on the social phenomena (weather, earthquakes, etc.) and the social activities (smart city, healthcare, etc.). In October 2019, Hexagon M.I. and Tokyo University of Science (TUS) signed a joint research to promote research on DT and smart manufacturing, infiltrate the core competency into Japanese manufacturing industries and develop human resources thereof. In April 2020, in order to increase the opportunities for interaction between academia and industry, Hexagon/TUS Digital Twin Laboratory (DTlab) was established at the Katsushika Campus of TUS [1].

As is well known, DT consists of three elements, *i.e.* a physical entity, a virtual counterpart, and the data connections in between. A widespread definition and extensive concepts about DT have been employed so far, and DT is conceived as a major tool in the manufacturing industry to carry out smart manufacturing, fault diagnosis, robotic assembly, quality monitoring, job shop scheduling, and decision making. The main enabling technologies for DT [2] can, in our recognition, be categorized into: (1) elemental level (*e.g.* physics-based modelling, data-driven modelling, big data cybernetics), (2) system level (*e.g.* infrastructure and platforms, human-machine interface.) Also DT can be divided depending on their applications: product DT, production DT, and performance DT. At the DTlab, the research of elemental level technologies was started initially particularly focused on the production DT phase where computational simulation is no doubt one of the keys, and high-fidelity physics-based simulation, multi-objective optimisation, design space exploration and data science approach including PCA, machine learning are being studied [1].

In this paper, the basic idea and background, and the aim of a strategic effort launched at the TUS DTlab in 2020 to infiltrate DT competency into Japanese manufacturing industries are first summarized. Next, some preliminary research results at DTlab are presented, for example, the numerical evaluation of the compression after impact strength for CFRP laminate with the help of X-ray CT image information, the numerical prediction of warpage in additive manufacturing, the indoor airflow analysis by CFD with a 3D as-built model based on the point cloud data obtained from 3D laser scanning, and the acoustic anomaly detection for predictive maintenance using machine learning. Finally, the future perspective on the DT joint research and the DTlab activities will be discussed including the idea of establishing a smart factory research centre which provides a place for practice of DT between TUS and the joint research companies.

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Real World Modelling beyond the Paradigm of Industrie4.0 and Society5.0

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Key Words: *Digital transformation, IoT, Industrie 4.0, Society 5.0, beyond the paradigm*

The digital transformation is one of the key challenges of, not only global product development and production, but also all areas of business processes. In addition to that, it also has a significant impact on every society and even each individual. Depending on the cultural and industrial background, this transformation has diverse effects on the different economic systems and areas, where the penetration of IT changes manufacturing systems, business processes and even people's lives for the better in every aspect.

For this digital transformation, there are two major paradigms which are on-going in the name of Industrie 4.0 and Society 5.0. Industrie 4.0 represents the forth industrial revolution that has occurred especially in manufacturing industries originally initiated by Germany. Industries 4.0 application includes wide areas, such as logistics, supply chain, autonomous equipment and vehicles, robots, additive manufacturing, IoT and cloud, opportunity identification, and so on. In the meantime, Society 5.0 covers human life activities as opposed to Industrie 4.0 covers manufacturing activities. Society 5.0 was proposed in the 5th Science and Technology Basic Plan as a future society that Japan should aspire to. It follows the hunting society (Society 1.0), agricultural society (Society 2.0), industrial society (Society 3.0), and information society (Society 4.0) [1].

These two paradigms seem to have differences in the focus of digital transformation: one targets industries while the other targets societies. However, when looking at these digital transformations from the viewpoint of interdisciplinary, connectivity, and network, there are many common issues where both countries are facing. Japan-Germany Symposium on IoT design, systems and applications, or JGIoT-DSA[2] is one of the academic platforms organized by the volunteers, where researchers from both countries discuss the issue from the different perspectives in terms of design, systems, and applications. As a result, this platform offers an meaningful and significant opportunity to discuss these issues and to propose a common solution to these two paradigms. This talk shares ideas regarding what is expected beyond the paradigm of Industrie 4.0 and Society 5.0, which has been discussed in this platform, and it also discusses real world modelling of cyber-physical systems beyond these paradigms.

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Development of Pre-evaluation Method for Applicable Points of Non-Target Image Displacement Measurement

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Key Words: *Railway Bridge, Image Displacement Measurement, Multipoint Measurement*

Displacement of a railway bridge due to the passage of a train is one of the typical performance indicators, and various measurement methods have been developed to realize efficient and quantitative maintenance. Displacement measurement with a video camera can measure multiple points at the same time, and there is a possibility that the curvature of bridge deflection, which is highly sensitive to damage, can be easily calculated. In previous studies, the accuracy of non-target multipoint displacement measurement of bridges by a video camera was verified, and it was shown that the displacement responses in the mid-span of a bridge can be measured with constant accuracy as the existing method [1]. However, there were some measurement points in the image where the displacement response could not be obtained due to overexposure points and so on [1]. For determining the curvature of bridge deflection, it was necessary to establish a method for pre-extracting such points. In this study, a new method to pre-extract measurement points suitable for displacement estimation is proposed.

The displacement estimation was premised on the use of the digital image correlation method, which calculates the amount of pixel movement by normalized cross-correlation (ZNCC). In addition, the sub-pixel estimation is based on the fitting of a quadric surface to 9 points composed of the maximum ZNCC pixel and the surrounding 8 pixels [1]. The purpose of this study is to make a simple evaluation as to whether such sub-pixel estimation is possible based on this premise. Authors focus on the second-order differential value at the maximum quadratic surface point used for subpixel estimation, and extract information on displacement estimation accuracy from the determinant of the Hessian matrix at each measurement point. To calculate the displacement response, multiple images that make up the captured video are required, however this method only uses the values calculated by sub-pixel estimation between the first and second frame images, which are the reference images.

As a result of applying the proposed method by continuously setting measurement points in the longitudinal direction of a main girder of a steel railway bridge, higher index values are taken at the position where the stiffener exists, and displacement response can be obtained at these higher index points. On the other hand, it was confirmed that displacement response could not be obtained at most of the measurement points where the determinant of the Hessian matrix had a value close to 0. In addition, the positions of these higher values have almost the same as those of the higher values of the variance of the luminance in the vicinity of the measurement point. This fact can indicate that displacement response can be easily obtained at a measurement point where the change in texture is large. By projecting obtained image information on measurement accuracy onto an image scheduled for video recording, it is possible to understand the points that can be used as measurement points before displacement estimation. This method can also be used to adjust the camera position, which is suitable for measurements with many displacement estimation points.

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Drive-By Bridge Quasistatic Deflection Estimation Using Track Irregularities Measured on a Passing Train

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Key Words: *Drive-by bridge inspection, bridge deflection, track irregularity*

Methods to estimate bridge frequencies and modal shapes using sensors installed on traveling vehicles are proposed as efficient bridge-monitoring methods [1] and have gained much attention as they enable drive-by bridge inspection [2]. One of the typical performance indexes of railway bridges is the deflection under train passage. If bridge deflections can be measured by the traveling vehicles, the time- and cost-intensive ground measurements can be avoided. In addition, measurement by traveling vehicles can greatly contribute to realizing quantitative and high-frequency condition evaluations. However, not much progress has been made in the field of bridge deflection evaluation based on on-board measurement data (acceleration of each vehicle part or track irregularity) in theoretical or experimental works.

This study aims to contribute to establishing this innovative drive-by bridge deflection estimation method. As the first step, a drive-by Bridge quasiStatic Deflection (BSD) estimation method was developed in this study. This method is based on the track irregularities of the first and last vehicle positions that are actually measured on a daily basis. Based on the measurement of the track irregularity of the front and rear bogie positions of one vehicle, theoretical examination revealed that the difference between these irregularities and the BSD are in a proportional relationship, and the proportionality coefficient depends only on the bridge span length and the load interval. In addition, it is clarified that this relationship can be extended to the track irregularities measured by the first and the last vehicles of a train with multiple vehicles. Thereafter, a method of estimating easily the maximum BSD when the train travels is proposed. This estimation is based on the maximum value of the difference between the track irregularities measured by first and last vehicles using a conversion coefficient corresponding to the span length.

The effectiveness of the proposed method was verified by numerical simulation. Thereafter, a correction coefficient was added according to the measurement method, such as string or chord length, of the track irregularity required for application to actual railways. Thereafter, the proposed method was applied to the track irregularities measured for the first and the last vehicles of an actual train traveling at a speed of about 100 km/h, and the BSDs on the railway line were estimated. Furthermore, the estimated values of six of these bridges were compared with the deflection measured from the ground during the passage of trains at a low speed. The results demonstrate that the proposed method measured the BSD with good accuracy within 10% error. This method was developed considering special conditions in which the dynamic response of bridges was ignored; hence, the applicable conditions are limited when the traveling train speed is low. Despite such drawbacks, this work makes a remarkable scientific contribution by paving the way for advances in drive-by BSD estimation via original theoretical and field studies.

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Identification Method of Higher-Order Local Vibration Modes Using Multipoint Excitation and a Reciprocity Theorem

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Key Words: *Rail Bridge, Modal Identification, High-Order Local Mode*

The local member vibration of steel railway bridges that occurs under train passages can lead to fatigue and structural noise. Existing research indicates that structural noise, in particular, adds to ambient noise in a wide frequency band from 100 to 2,000 Hz in I-girder open steel railway bridges with directly connected tracks. However, the mode shapes of the higher-order vibration mode that is the source of such structural sound are more complicated than those of the lower order and have several nodes in the same member. Therefore, to evaluate the predominance of high-order local vibration modes and this contribution to structural noise under train passages, the mode shapes of the local vibration mode in the actual bridge must be identified. Nevertheless, a large-scale multipoint measurement that can identify complex vibration mode shapes cannot be applied to field tests with high temporal and spatial constraints. Thus far, few examples have been given concerning the identification of high-order local vibration mode shape of railway bridges that exceed 100 Hz.

The present research proposes a new method for identifying the frequencies and mode shapes of the local vibration modes of steel railway bridges using field tests. This method significantly reduces the time and labor required to install a sensor using multipoint excitation with an impulse hammer instead of multipoint measurement. Furthermore, by exchanging the relationship between the input and the output points that are obtained as transfer functions based on Maxwell's reciprocity theorem, the vibration mode can be identified based on a simulated large-scale multipoint measurement. In addition, the method includes an entirely original phase-referenced procedure that corrects for the slightest phase synchronization error between the hammer and sensor, which is crucial in the reciprocity theorem.

The proposed method was applied to a steel I-girder bridge with a span length of 20 m. The frequencies and mode shapes up to around 1,000 Hz of the steel bridge main members such as the upper flange, web, lower flange, and stiffener for one panel (approximately 1,000 mm in the longitudinal direction) separated by the stiffeners were identified using a multipoint hammering test. In particular, on the web, it was found that high-order complex vibration modes, such as vertical 7th order and horizontal 3rd order, which had previously only been identified using theoretical analysis, also exist in actual bridges. Moreover, a comparison with an existing identification method based on multipoint measurement and theoretical calculations confirmed that the proposed method could identify the frequencies and mode shapes of the members with a high level of accuracy. Subsequently, the identification result was compared against the measurement spectrum when trains passed; the local member vibration modes, which can be the source of the structural noise, were identified. Furthermore, it was suggested that the specified vibration modes vibrate significantly when a train passes owing to the coincidence with an excitation frequency that is caused by periodical track irregularity.

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Method for Identifying High-order Local Vibration Modes of a Steel Railway Bridge

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Key Words: *Steel Railway Bridge, High-order Local Vibration Mode, Modal Identification*

The local member vibration of steel railway bridges that occurs when a train passes can cause fatigue damage and structural noise. In particular, rail joints on steel bridges may cause fatigue damage due to the introduction of impact forces with high frequencies and the corresponding Higher-order Local Vibration Modes (HLVMs) of steel bridges [1]. However, mode shapes of HLVM are more complicated than those of the low order modes, and have many nodes in the same member. Therefore, in order to evaluate the effect of HLVM, it is necessary to identify the mode shape of the HLVM in an actual bridge. However, large-scale multipoint measurement that can identify complex vibration mode shapes cannot be applied to field tests with large temporal and spatial constraints. So far, there have been few HLVM identification results of railway bridges exceeding 100 Hz [2]. In addition, the modal damping ratio, which greatly affects the repetition of HLVM, is an open problem that has not yet been clarified.

In this study, a novel identification method for frequencies, mode shapes and the modal damping ratio of the HLVMs of steel railway bridges was developed. The proposed method consists of the following four contents: 1) multi-point excitation with impulse hammers instead of multi-point measurement, 2) Maxwell's reciprocity theorem [2] for exchanging input points and output points, 3) estimation of multipoint free vibration by back calculation from transfer functions and 4) modal identification by ERA method from estimated multipoint free vibrations.

The proposed method is applied to a steel I-girder bridge with a span length of 10 m, and the HLVMs up to about 1000 Hz of upper flange, web, lower flange, and stiffener for a panel (about 600 mm in the longitudinal direction) separated by a stiffener have been identified. Since the number of measurement points has increased significantly due to multi-point excitation compared to the conventional measurement method, it is clearly shown that the mode shapes of HLVM with a complicated shape can be precisely identified. In addition, the modal damping ratio of the identified HLVMs indicated low values of around 1% in many modes. This means that the vibration duration of the HLVMs can be long. In other words, it is suggested that it may have a great effect on repetition in fatigue damage. The obtained results provided important basic information in the fatigue evaluation of steel railway bridges considering the influence of HLVMs.

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On situ vibration based structural health monitoring of a railway steel truss bridge: a preliminary numerical study.

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Key Words: *Steel truss bridge, railway bridge, structural health monitoring, direct monitoring, vibration-based monitoring.*

Viaducts and bridges enable daily transportation of goods and passengers throughout the entire country. Railway network is subject to increasing travelling loads and traffic frequency. In addition, most of the bridges were built in the last century: they are subject to ageing and degradation [1], as an unavoidable phenomenon. It is therefore necessary to develop proper structural health monitoring systems that can support periodical visual inspections. That is why infrastructure managers are always looking for new technologies to assess in an almost continuous way the health status of their network components. Direct monitoring systems consist of mounting a set of different sensors on the structure under analysis, whose measurements are then used in order to assess structure mechanical performances and status. Given the nature of the bridge/viaduct to monitor and the kind of damage to detect, it is important to choose the proper typologies of sensing devices. Moreover, the following step is represented by the choice of an adequate damage-sensitive index (or set of them), that is able to capture and reflect eventual changes in structure performances during time. This paper is the result of a numerical study performed on a 3D FE model based on an existing structure: the studied bridge is a Warren truss railway bridge, located in Northern Italy, built few year after the second world war. The authors investigated the performances of different vibration-based methods [2]-[3], namely two modal-parameters based approaches and a non-modal ones. The former, based on the use of modal parameters (natural frequencies and mode shapes) as damage-sensitive indexes, was shown to be slightly sensitive to damage, also applying important flaw intensities. Instead, the latter, that do not imply the computation of any modal parameter, showed better results, both in terms of damage identification and localization. In particular, exploiting the RMS values of the signals recorded by a mesh of velocimeters placed along the span can represent a possibility to detect damage presence and its approximate location. This analysis has been performed for a set of different damage scenarios, suggested by the infrastructure managers. The simulations were run adopting a complete multi-body train model. Furthermore, in the attempt to get closer to real operating conditions, the actual track profile featuring the considered line portion was inserted in the simulation program.

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15th World Congress on Computational Mechanics (WCCM-XV)
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A Study on Three-Dimensional Structure of a Wind Turbine Wake Using Computational Fluid Dynamics

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Key Words: *Mutual interference of wind turbine wakes; Reynolds-Averaged Navier-Stokes (RANS); Doppler beam swinging (DBS) Light Detection and Ranging (LiDAR)*

In order to promote introduction of a large-scale offshore wind power generation system, it is necessary to accurately evaluate the wind conditions at sea and optimize the wind turbine layout in a wind farm. In a wind farm consisting of multiple wind turbines, the effects of upstream wind turbines cause wake where spatial and temporal variations of wind speed occur. Therefore, it is essential to correctly evaluate the influence of upstream wind turbines on the wind conditions in the wake and to determine the separation distance between wind turbines. We have been conducting joint research with the Institute of Applied Mechanics, Kyushu University and Hitachi Zosen Corporation since 2018 to develop a versatile wake model [1].

In the wind turbine wake region, there are velocity distributions in both horizontal and vertical directions. It is important to understand this characteristic, and in this study, we used computational fluid dynamics (CFD) to clarify the three-dimensional wind speed distribution in the wake region. The CFD simulation base on the unsteady Reynolds-averaged Navier-Stokes (RANS) equations was performed. The simulation indicates that wind speed vector in a wake region shows complex changes.

In order to verify the accuracy of the simulation, we carried out measurements of the wake at a wind power plant site by using Doppler beam swinging (DBS) Light Detection and Ranging (LiDAR). The single LiDAR unit measures the wind speed distribution in the vertical direction at the LiDAR placement location and cannot evaluate the wind speed distribution in the horizontal direction. To measure the wind speed distribution in the horizontal direction, simultaneous measurements using two LiDAR units were performed. One of them was set along the inflow direction and another one was set with 45 degrees rotation. From the results of the comparison between the simulation and the measurement, it was confirmed that the simulation do not agree with the trend of the measured results for sea wind. On the other hand, the simulation agreed with the trend of the measured results for the land wind.

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Consideration of the Behaviour of a Wind Turbine Wake Using High-Fidelity CFD Simulations

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Key Words: *Wind turbine wakes, Large-eddy simulation (LES), Actuator line model, Wind direction fluctuations*

During a wind turbine is in operation, a wake is created behind the wind turbine and it reduces the power generation and lifetime of a wind turbine located downwind. Therefore, it is important to accurately predict the effects of wake in order to assess the feasibility of a wind farm. Hitachi Zosen Corporation has been conducting joint research with the Institute of Applied Mechanics, Kyushu University and Toshiba Energy Systems & Solutions Corporation since 2018 to develop a versatile wake model [1]. In this paper, we report the three-dimensional structure of the unsteady wind turbine wake and the behaviour of the wake when wind direction variation is given to the inflow wind, obtained by numerical simulation of the Omonogawa wind power plant conducted during the development process.

We conducted numerical simulations to reproduce wind turbine wake using the "RIAM‐COMPACT" real urban version [3]. The following findings were obtained from the simulation results. Inside the wake in 1D downstream of a wind turbine, a flow field that rotates in the direction opposite to the blade rotation direction occurs. There is no significant difference in the flow field of the wind turbine wake between the up-wind type and the down-wind type. In 5D downstream of a wind turbine, the vertical distribution of the mainstream velocity component is almost the same regardless of the power of the inflow profile in the swept area of the wind turbine. When the inflow wind has a wind direction variation defined by a sinusoidal function with a maximum value of 10 degrees, the wind turbine wake is quite diffuse and the results of its vertical profile are in good agreement with the field measurement results by a vertical profiling lidar.

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Design of wind turbine blades made of carbon fiber composite material and examination of reinforcing fiber types

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Key Words: Industrial Applications, Multiphysics Problems, Fluid-Structure Interaction, Wind Turbine

The construction of offshore wind farms where it is easy to obtain stable winds in large areas is becoming more and more active. Since the efficiency of a wind turbine is proportional to the cube of the wind speed and the square of the blade length, wind turbine blades built in the farms have been getting enormous in recent years. In order to realize larger wind turbine blades in the future, it is necessary to design lighter and stronger wind turbine blades. This study performed fluid structure interaction (FSI) analysis [1] combining a multiscale structural analysis, a three-dimensional unsteady fluid analysis around the wind turbine blade, and structural sizing based on the FSI analysis result. We investigated the influence of the material properties of CFRP reinforced fiber types on the design solution in terms of the thickness and weight of the wind turbine blade.

Fig. 1 Phase averaged non-dimensionalized pressure p^* distribution on blade [2] surface $(0.61 \leq p^* \leq 0.65)$.

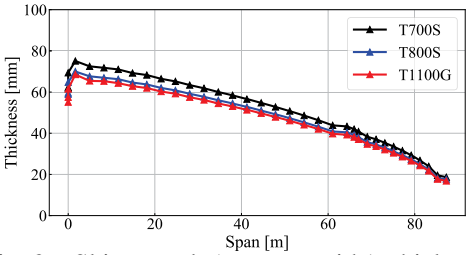

Fig. 2 Skin panel (pressure side) thickness along blade [2] span.

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Developments in Wind Turbine Wake Modeling based on Machine Learning

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Key Words: *Wind Turbine Wake, Machine Learning, CFD, Lidar, Wind-tunnel*

This study provides a development of a new wind turbine(wake) modelling method based on machine learning for precise wind prediction by numerical simulation. (wake: Area where the wind speed generated on the downstream side of the wind turbine is low, and the airflow is complicated and turbulent.) Evaluation of site-specific wind conditions is required in wind power since turbulence is cause of wind turbine failure, although wind is source of energy. In a large-scale wind farm consisting of multiple wind turbine groups, the interaction of "wake" between wind turbines causes a decrease in the total power generation and an increase in the risk of failure. Therefore, in the wind power generation business, it is important to select the optimal installation site taking into account the effects of wakes, the optimal design of the wind turbine layout, and the operation of the power plant with minimal risk of failure.

Wind simulation has been utilized in the design and operation of wind farms. These simulations enable highly accurate prediction of power generation and evaluation of the risk of wind turbine failure by precisely reproducing the reduction in wind speed and wind turbulence caused by wakes, together with meteorological and oceanographic characteristics and topographic turbulence. In the field of wind simulation, a number of physical models (wake models) have been proposed and validated to reproduce wakes with high accuracy. Uchida et al. [1] succeeded in developing a CFD porous disk model, which simulates a part of a wind turbine rotor with a resistive element, and demonstrated its effectiveness by comparing it with actual measured data of wind farms in coastal areas. In recent years, however, expectations for new modeling methods based on machine learning have been rising. Machine learning has the potential to accurately model complex nonlinear phenomena that are difficult to formulate, such as wakes. In this study, we constructed and verified the accuracy of a new wake model using machine learning, which is different from the conventional fluid dynamics viewpoint, in order to realize a wake model with high robustness and versatility that does not require complicated parameter adjustments. For the supervisory data of the machine learning model, we used wind tunnel tests, LiDAR measurements for coastal wind turbines, and time series data during the inflow wind speed and wake region from the CFD analysis (without modeling the wake). These measurements and analyses produce a variety of wind data sets at different wind turbine outputs (blade lengths) and wind conditions.

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Validation of Wind Prediction Accuracy of Wind Flow Simulation Based on LES Considering Atmospheric Stability at a Developing Offshore Wind Farm Affected by Topography

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Key Words: *Offshore Wind Power, Topography, CFD, LES, Atmospheric stability*

In recent years, there have been calls for the expansion of renewable energy both in Japan and abroad, and bidding for offshore wind farms has begun in Japan. In Europe, many offshore wind farms have already been installed, but in order to accelerate the introduction of offshore wind power in Japan, Japan's unique problems must be solved. In Europe, offshore wind farms are more than 10 km from the coast, whereas in Japan, offshore wind farms will be only a few km from the coast because the water depths deepen near the coast. As a result, the site will be strongly influenced by the onshore topography, and the wind speed distribution in the site may not be uniform and the turbulence intensity may be high. In addition, it is known that airflow separation due to topography is affected by atmospheric stability [1], but there are very few studies on how atmospheric stability affects offshore sites in Japan, since atmospheric stability varies with region and season. In order to solve these problems unique to Japan, it is essential to verify the accuracy of wind flow simulations that can reproduce the effects of topography and can be set to any atmospheric stability level, rather than just the conventional atmospheric stability neutral.

In this study, the annual frequency of atmospheric stability and the effect of topography were investigated using ERA5 data and observation data from wind observation masts installed at four locations on the island for a site under development where bidding will soon begin. As a result, it was found that a variety of atmospheric stabilities appeared at the site and that the annual average events were not neutral but unstable, and the deviation from neutral varied depending on the season and wind direction. The turbulence intensity varies greatly depending on the mast position and wind direction, and it is necessary to reproduce the wind flow separation due to topography in order to predict the wind conditions of wind turbines located close to the island. The accuracy of the wind flow simulation by LES was verified using the mast-to-mast wind speed ratio. As the simulation software, we used the commercial Riam-Compact [2], which is widely used in Japan, based on which the atmospheric stability can be arbitrarily set. As a result, it was found that the accuracy could be improved by refining the analytical wind direction classification and taking the average of the results calculated with several atmospheric stability levels.

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A Particle-Based Simulation for Friction Prediction of Rubber on Snow

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Key Words: *Material Point Method, Coupling Methods, Snow Simulation*

In order to develop tires that can run safely even on snowy road, it is necessary to elucidate the complex frictional phenomena between tires and snow. Since it is difficult to elucidate this mechanism through experiments alone, it is necessary to apply prediction technology. Since the properties of snow vary depending on a variety of factors, prediction technology that can reproduce the differences in snow behavior is needed. Finite Element Method (FEM) [1] based on the Lagrangian formulation is commonly applied for deformation analysis of tires. However, if FEM is applied to snow, large deformation of snow distorts elements. Therefore, in order to solve the complex interaction between snow and tires, Material Point Method (MPM) [2] is applied to predict snow deformation in this research.

MPM is a particle method based on continuum mechanics. Physical quantities such as stress and strain are placed in the particles, and the equations of motion are solved by a grid placed in the background. MPM is suitable for large deformation analysis, and there are examples of its application to snow simulation [3].

FEM can change the resolution of the analysis by changing the size of the elements, but MPM is difficult to change the resolution of the analysis. Therefore, modeling both tires and snow with MPM requires a huge amount of calculation time. Therefore, FEM is applied to tires, and MPM is applied to snow.

Tires have designed grooves called a tread pattern, which affect the traction performance of the tire on snow. As a fundamental research for the development of tread patterns with higher traction performance, the coupled MPM-FEM method was applied to predict the friction prediction on snow of rubber blocks. The prediction analysis was performed under different conditions of snow properties and rubber block shapes, and was verified by comparing with experiments.

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A study on Prediction of Water Discharge Performance for Showerhead Product Design

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Key Words: *Showerhead, finite volume method, MPS particle method, fluid splash, droplet, mixing, product design*

LIXIL Co. handles a wide range of water-related products such as toilets, baths, and kitchens. The fluid behaviour control is a key technology for developing of these products. Therefore, the numerical simulation with CFD plays an important role in product and technical development.
The flow of water in a toilet has been simulated with the finite volume method (FVM). However, the simulation with a large number of fine droplets such as in a shower needs a lot of computational cost. To deal with this problem, MPS particle method[1] has been introduced to take advantages of enabling for simulating such as liquid splashing, and mixing. In this paper, the application of the simulation to the design of a showerhead is discussed.
The discussed shower has high water-saving performance. The impeller inside the showerhead rotates at high speed while half blocking the holes in the showerhead. By increasing the pressure in the blocked area, strong water flows can be released even with a small amount of water. This enables a bathing experience with a sense of water volume while maintaining high water-saving performance. The possibility with the MPS for product development was investigated for this shower, too.
The major subjects to be studied are as follows;

(1) Prediction of impeller rotation speed and transition
(2) Prediction of water behaviour and droplet size
(3) Prediction of internal pressure of the showerhead

In conventional MPS particle method, the accurate prediction is difficult because an only constant rotational velocity can be applied to the impeller. To improve the accuracy, it is necessary to solve the problem by coupling the water flow and the motion of the impeller. Therefore, in this research, a coupling technique of MPS and rigid body dynamics are applied. As a result, the simulated results show a good agreement with the experimental one.
This paper focuses on the application of the MPS particle method to the showerhead design. Since computational efficiency is also an important factor for the product development, the computational performance of multi-GPU for the MPS particle method is also discussed.

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Applications of Particle Method to Fine Particle Dispersion System

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Key Words: *Fine particle dispersion system, Shear flow, Moving particle semi-implicit*

It is industrially important to understand the flow properties of materials containing multiple components such as particle dispersion in liquids and droplets. For example, controlling the rheological properties of the slurry solution is effective in battery development and clarifying the evaporation mechanism of ink droplets improves image quality of the inkjet printer.

In these fine particle dispersion system, the experimental study is difficult because the size of particles is so small (ranged from nm to μm) and particles interact intricately with each other. In these situation, simulation methods for such systems have been studied recently. SPM(Smoothed Profile Method) has been developed and applied to analyse the motion of dispersed colloidal particles in a shear flow [1] and SPH(Smoothed Particle Hydrodynamics) with lubrication force model has been studied for shear-thinning phenomenon [2].

We develop a method based on MPS (Moving Particle Semi-implicit) [3] to analyse the rheology of the fluid with dispersed particles in a shear flow. The algorithm and some applications to the fine particle dispersion system will be discussed in our presentation.

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Particle Accretion Simulation Using Particle/Grid Hybrid Approach

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Key Words: *Multiphysics Phenomena, Particle Method, Accretion, Industrial Application*

In manufacturing processes and in the operation and maintenance of industrial products, the accretion of foreign matter in products affects performance, the creation of defects, maintenance periods, etc. Therefore, it is necessary to have techniques to predict where accretion will occur and the amount. There are various examples of accretion phenomena such as dust in inspection apparatuses, carbon accretion in automobile engines, frost on the heat exchangers of air conditioners, and snow on the bogies of high-speed trains. In this study, a simulation for predicting snow accretion on high-speed trains was developed as a common technique for the above problems. Allain et al. [1] developed a snow-accretion simulation for high-speed trains. Snow was modeled as spherical particles, and an Euler-Lagrange approach was applied to simulate the interaction between snow and air. The snow concentration in the air was assumed to be small enough to have no significant influence on the solution of the flow field. The ratio between the mass flux of the simulated particles and the real mass flux was used to estimate the actual snow-accretion mass. Murotani et al. [2] developed a snow-accretion analysis method that reproduced snow-accretion growth processes. Snow was also modeled as a sphere, and the boundary shape, modified by the snow-accretion form, was reflected in the boundary shape of an air flow simulation. The approach was validated with a snow-accretion experiment on a cubic model, and the results agreed well with the snow accretion in the experiment. These two studies demonstrated excellent approaches that are highly accurate and practical. However, a lot of particles are needed to obtain statistical homogeneity, so this factor increases the computational load. In this study, we developed a particle-accretion simulation with a small number of particles in order to reduce the computational load. A particle/grid hybrid approach that was previously developed [3] was applied. In the simulation with grids, a two phase flow that consisted of dry air without snow and wet air with snow was simulated. Snow behavior was simulated by using parcel particles containing snow particles with the same diameter and same velocity. The parcel particles were uniformly generated only in the wet air around observation areas, so it was possible to significantly reduce the number of particles. The wall accretion of the parcel particles was controlled on the basis of the velocity and angle between the velocity and normal vectors at the wall surface. The developed simulation approach was first validated with snow accretion on a cubic model [2], and the simulated accretion shape agreed well with the measured one. Furthermore, the simulation approach was applied to snow accretion on bogies of a high-speed train with three bogies. Qualitative and reasonable results regarding the location of snow accretion were obtained.

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Simplified Heat Transfer Modelling of Impingement Cooling Using Particle-Based Method

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Key Words: *MPS method, Impinging Jet Cooling, Heat Transfer Coefficient, Rotating Machinery*

The realization of high cooling performance for oil-cooling electric vehicle (EV) motors is energetically promoted. It is very important to comprehend the characteristics of oil flows and the impingement cooling in the development. It is promising to utilize the MPS method [1], which is one of particle-based methods and suitable for free-surface flows with moving walls, for oil-impingement cooling analysis in EV motor development. However, it is difficult for the particle-based method to increase the resolution near the component surface as in the conventional mesh-based method. In the MPS method, this makes it difficult to evaluate the heat transfer between the component and the fluid, that is, to utilize it for the thermal design of EV motors.

In the present study, the heat transfer coefficient model suitable for the impinging jet flow, which is important in the thermal evaluation of oil-cooling EV motors, is constructed [2]. The local heat transfer coefficient is obtained by the model corresponding to the stagnation area of the impinging jet flow and substituting the flow velocity and length scale near the component surface into the heat transfer coefficient correlation. The parameters included in the model are determined by comparison with the impinging jet flow experimental correlation.

The oil-cooling rotor calculations are conducted using the MPS method and model parameters, in order to simulate the local heat transfer coefficient of the rotor surface. The numerical results are compared with the experiment, and it is confirmed the heat transfer is satisfactorily reproduced with the present method.

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Hybrid Parallelization of Microscopic Traffic Simulator

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Key Words: *Traffic Simulation, Parallel Computing, Multi-Agent System*

Traffic policies, such as changes in the road environment, are costly to implement. Therefore, it is necessary to evaluate the traffic policies quantitatively in advance. For this purpose, it is appropriate to test the policies virtually using a traffic simulator. On the other hand, since traffic phenomena are complex systems, their prediction requires a high computational cost. Therefore, it is desirable that the simulator is not only accurate and scalable, but also optimized to be handled by a large-scale parallel computer.

In this research, we have attempted a hybrid parallelization of a multi-agent-based traffic simulator [1] using MPI/OpenMP. In this simulator, cars are modelled as autonomous agents. Each car's agent obtains information about its surroundings (position of other cars and traffic signals), makes autonomous decisions, and acts accordingly. In previous research, MPI parallelization has been achieved by dividing the road network so that the load is approximately equal and assigning it to each processor [2].

However, when using SMP clusters, hybrid parallelization can perform better than pure MPI parallelization in some cases [3]. Additionally, when using supercomputers, the number of MPI parallels may be limited. Therefore, in order to run a traffic simulator on a large-scale parallel computer, the authors perform hybrid parallelization of the simulator. The results will be presented at the conference.

Our approach contributes to the introduction of methods that have been used in the field of computational mechanics to the new field of social simulation.

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Improvement of Dynamic Hybrid Traffic Simulation Model to Expand Its Applicability

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Key Words: *Traffic simulation, Hybrid model, Cell transmission model, Intelligent driver model, Traffic Forecasting*

Traffic congestion is causing economic and environmental problems. Recently in Japan, road maintenances for roads used for a long time have been required in many places. Thus, a maintenance schedule that can minimize the effect of a traffic jam or any other social problems is necessary. Traffic simulation is useful for testing many scenarios at a low cost and finding a good maintenance plan.

In order to achieve both precision and low computational cost simultaneously, Takahashi et al. [1] proposed a dynamic hybrid traffic simulation model that uses different simulation models of different granularity, depending on the traffic condition and properties of road networks. In this approach, the Cell Transmission Model (CTM) [2] is employed as a macroscopic model regarding traffic flow as continuum fluid, while the Intelligent Driver Model [3] and MOBIL [4] are employed as microscopic models simulating the individual behaviors, are employed. The models are switched to each other dynamically during a simulation.

The main target area of this hybrid model is a highway, and the validation was conducted using real traffic data on highways. The results show that the model can perform accurate simulations with low computational costs. However, this model still has some limitations in the accuracy under certain situations and cannot model merge and diverge sections. To overcome limitations in the previous dynamic hybrid traffic simulation model, the authors in this study propose an improved model with higher accuracy and wider applicability. The concrete results of the study are to be reported at the conference.

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Simulation Framework Development for the Interaction between Road Traffic Network and Power Distribution System

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Key Words: *Electric vehicle, charging, coupled simulation, OpenDSS, MATES*

There is a worldwide demand for a sustainable carbon-neutral society, and the reduction of energy consumption derived from fossil fuels is an urgent issue. In the transportation sector, which accounts for a large percentage of energy consumption, the use of EVs (Electric Vehicles) with high environmental performance has been rapidly increasing in recent years. EVs are expected to play a major role in realizing a carbon-neutral society.

In this study, we proposed a coupled simulation framework that can represent the interaction between the transportation system and the power system. This will enable us to evaluate the impact of the introduction of EVs into society and to study the appropriate charging control policy. The framework is verified in a simple numerical environment, and it is shown that the two-way coupling can be executed correctly. In the proposed simulation framework, OpenDss [1] is used to simulate the power distribution mechanism, and MATES [2] (Multi-Agent Traffic and Environment Simulator) is used to simulate the road traffic mechanism. These two simulators run independently, but exchange information with each other through two-way coupling. MATES can link not only EV charging events but also congestion estimates and reservation status of charging facilities to OpenDSS. After power flow calculation, OpenDSS can link the rated output of chargers, rate settings, and other information to MATES.

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The Effect of Air Traffic Simulator Fidelity on Flight Delay

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Key Words: Air Traffic Management, Air Traffic Flow, Simulation Evaluation, Modeling Fidelity

Modeling the air traffic flow and evaluating the operational impacts have been widely conducted for the enhancement in the efficiency of Air Traffic Management. This paper investigates the effect of the fidelity of the simulation models on flight delay at a microscopic scale by comparing AirTOp commercial simulator and our proposed Cellular Automaton(CA)-based simulator; both are utilized in our previous studies [1, 2]. Our CA-based simulator[2] has been modeled to assess airport and airspace complexity at a macroscopic scale. On the other hand, AirTOp[1] can take into account the microscopic behavior of the aircraft by the new sequencing and spacing operation, so-called Point-Merge (PM) operation, started from 2019 at Tokyo International Airport (RJTT). In this study, both simulators model 578 arrivals at RJTT, consisting of 435 flights coming from south-west direction and 143 flights coming from the north direction. The actual data including radar track, and flight plans (FP) during the 6 months between September 2019 and February 2020 are analyzed to make 39-days traffic scenarios. Each agent (flight) departs reference points located in 200 NM from RJTT in south-west direction and 120 NM from RJTT in north direction and flies along the designated FP. The main difference exists in the spacing adjustment algorithms. AirTOp realizes the spacing adjustments by ”vectoring (taking a detour)” following the actual PM-operation. In contrast, the CA-based model implements spacing adjustments following 3 simple rules regardless of the area. As the result, the comparison reveals that AirTOp simulator captures the characteristics of the delay originated from PM-operation better than SBCA owing to the configuration of vectoring zones and the implementation of the actual speed and altitude restriction at PM-operation area. However, the results show that the calculated macroscopic metrics such as descent and speed profile, total flight time, total traveling distance, and separation at the runway threshold are well fitted to the actual operational data in both simulators. These findings suggest that air traffic simulators could deal with the delay area and amount in detail by considering the constraints of the location, speed, and altitude of sequencing and spacing.

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A Doubly-Asymptotic FEM Algorithm for Estimating the Ultimate of a Sequence of Increasingly-Dense-Meshed Finite Element Solutions[#]

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Key Words: *Asymptotic solution; finite element method; logistic function; nonlinear least squares method; statistical analysis; uncertainty estimation; verification.*

By considering every finite element method (FEM) solution [1] as the result of a numerical experiment for a fixed model, a purely mathematical problem, i.e., solution verification, can be addressed by first quantifying the errors and uncertainties due to their sources, and then developing numerical algorithms to assess the solution accuracy of all candidate solutions. In a recent paper [2], we presented a new approach to FEM verification by applying two mathematical methods, namely, (1) a 4-parameter logistic function to represent the behavior of an asymptotic solution of a specific FEM model, and (2) the nonlinear least squares method [3], to find the asymptotic solution and its 95 % confidence bounds. Using the two methods, we developed a numerical algorithm, to be known as "Asymptotic-FEM Algorithm (AFA)," we estimated an asymptotic FEM solution and its uncertainty at some very large degree of freedom such as one billion or more, based on the availability of a sequence of increasingly-dense-meshed solutions of a specific FEM model. Since a full logistic function has four parameters, we needed a minimum of 5 FEM candidates in the first sequence of increasingly-dense-meshed solutions to get one convergent asymptotic estimate. As the size of the sequence increases, we get more asymptotic estimates until when the size reaches 9, we get a total of five asymptotic estimates. In this paper, we develop a doubly-asymptotic FEM algorithm (DAFA) by applying the AFA again to the sequence of 5 asymptotic estimates in order to obtain an ultimate estimate of the solution of a specific FEM model. Our results include calibration of this DAFA method using problems of known analytical solutions and the application of the method to sample problems, of which no theoretical solution exists.

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Development of Efficient FEM Analysis Method using Equivalent 2D Model for Linear Friction Welding Analysis

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Key Words: *2D Model, Linear Friction Welding, High-Tension Steel, Solid Phase Bonding*

Linear friction welding(LFW) is one of the methods in accordance with the SDGs in machine-parts production processes. Lately the method has been used for not only airplane production but also automobile production owing to its rationality.

In the LFW process two machine-parts are bonded with their surfaces in solid phase with the friction-heat brought by lateral oscillation with each other. It needs neither big facilities like large electric energy sources nor other materials as in the arc welding.

But when the LFW analysis are planned the analysis models are usually prepared in 3D models. That is because LFW processes include 3D loads and 3D deformations. And accordingly the model becomes so big that it takes much calculation time and long development period.

We intended to develop 2D model for this analysis with the following method. In the LFW process small pressures normal to the friction surface are occurred through the lateral oscillating motions of the blanks. These pressures are important but lost in the 2D model.

We introduced the body-force field representing the upper-mentioned pressures in the 2D model. And the body-force field is generated by the centrifugal force on the blank considering that the pressure-forces are independent of the push force of the blanks.

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Development of Mold Filling Process Simulation considering Air Entrainment using SPH Method

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Key Words: *Particle Method, SPH, Die Casting, Air Entrainment, Mold Filling, OpenMP*

Die-casting is a casting method suitable for mass production because it can accurately form complicated shapes. However, when the mold is filled with the molten metal, there is unsatisfactory performance that casting cavities (gas porosity) are generated due to air entrainment, and the strength of the product varies.

Recently, with the aim of improving the quality and production efficiency of castings including this air entrainment, there has been many studies of simulating the behavior of molten metal during filling and visualizing the state of gas entrainment using CAE.

In this study, the mold filling process considering air entrainment in the die cast are simulated using the two-phase flow SPH method, that can be applied to the mold flow including gas entrainment[1], [2]. Then, the behavior of air entrainment due to the filling of molten metal (Aluminum alloy), especially the efect of injection speeds are investigated.

The particle model (number of particles: 270,000) that simplifies the 3D die-casting shape in the field is used in this simulation. And particles with a specified speed flow in continuously at the molten metal inflow gate. At the outlet (vent part), particles flowing out of the mold are erased.

In concluson, it is possible to investigate/visualize the air entrainment behavior at the time of filling the molten metal and the flow behavior due to different filling speeds, which is considered to be effective for improving the gas porosity of the cast product.
In addition, to speed up the two-phase flow program by SPH method, a parallel algorithm using OpenMP, which enables parallel calculation on a shared memory type machine, has been implemented. As the result of parallel calculation, we were able to achieve more than 3 times faster computational speed on a PC with 4 cores.

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Development of two-phase flow simulation using SPH Method

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Key Words: *two-phase flow, SPH, foundry filling process, air entrainment*

Gas entrainment is one of the major defects caused in the foundry filling process. Since the smoothed particle hydrodynamics (SPH) is a Lagrangian method that does not use a lattice, large deformations and movements can be easily analyzed, so it has the potential to be applied to such gas defect prediction as a methodology. However, numerical simulation of the two-phase flow, in particular those with large density ratio, has been challenging. It is because the discontinuities of the density and the sharp pressure gradient exist over the interface. Authors have developed a two-phase flow SPH methodology that can be applied to the foundry filling process containing gas [1].

The weak compressible SPH(WCSPH) was used as the analysis method. Strictly speaking, water has a slight compressibility. The weak compressible SPH is solved by using NS equations and equations of state (EOS) alternately. The Tait equation was used for EOS.

The methodology developed in this study is applied to bubble rising in water, which is a typical problem of gas-liquid two-phase flow. The bubble / water density ratio is 1/1000. In the 2D as well as 3D calculation results for the bubble radius 20 mm, the bubble shape became a spherical cap as shown by Grace [2]. The water tests regarding the gas entrainment in the inclined part of the rectangular cavity and air exhaust from backstep part were also analized. Good agreement between the water tests and simulation results demonstrates the success of the SPH methodology development.

The methodology in this study is applied to the 3D mold filling process simulation considering air entrainment [3].

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A New Forest Evapotranspiration Model Accounting for the Spatial Variability of Rain-snow Fraction and Forest Conditions

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Key Words: *Evapotranspiration, Rain-snow fraction, Forest conditions,*

Evapotranspiration (ET) is one of the most important hydrological processes in forested catchments and is essential in terms of water resource management. ET differs depending on the precipitation type (rainfall or snowfall) and forest conditions, such as, species, stand density, and tree height. For example, rainfall interception ranged 10–20 % of the rainfall, while snowfall interception ranged 30–50 % of the snowfall in evergreen coniferous forests. In addition, rainfall and snowfall interception ranged 10–40 % and 0–10% of the rainfall and snowfall in deciduous broadleaved forests, respectively. Thus, our objective in this study is to estimate catchment ET based on the new practical model which accounting for precipitation types and forest conditions.

Our new model was based on the model developed by Komatsu (2020). In particular, the part of interception loss (Ei) needed to be improved in terms of different precipitation input (rainfall and snowfall). Ei was estimated by species, stand density, and tree height as Ei rate to precipitation based on the review of 77 published studies all over the world. Transpiration (Et) and forest floor evaporation (Ef) were estimated by species, stand density, tree height, and climatic data. We further applied the model to three forested catchments located in Ymanashi Prefecture, central Japan (area: 21km^2, elevation: 680 to 2200 m a.s.l.).

Estimated annual rainfall Ei ranged from 64 to 460 mm with a mean of 282 $\pm$ 100 mm and snowfall Ei from 18 to 241 mm with a mean of 47 $\pm$ 42 mm. Annual evaporation from dry canopy (i.e., Et and Ef) ranged from 190 to 1034 mm with a mean of 507 $\pm$ 186 mm. The total ET ranged from 412 to 1195 mm with a mean of 809 $\pm$ 206 mm. We found the different distribution of ET in each of the catchments and which was caused by the forests and meteorological conditions depending on altitude and management history. Incorporating our model with LiDAR remote sensing, we can estimate the distribution of ET within catchments and thus it can be effective for future catchment management.

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Integrated Study on Groundwater Utilization System at Water Outage/shortage during post-Disasters and or Draughts: Watershed Modeling and Scenario Analysis

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Key Words: *Integrated Watershed Model, Water Outage, Groundwater Utilization System*

In emergencies such as large-scale earthquakes, floods, and accidents, "water outage" is still the most familiar and urgent problem. In the questionnaire "Problems after the disaster", "Securing sufficient water" always ranks high. In the event of a large-scale earthquake in the past, not only will it have a major impact on domestic water, but it will also become a bottleneck for resuming operations due to the total water outage of industrial water, and it hinders rapid recovery and rebuilding of life. In the report of the National Land Council in May 2017, "About the ideal water resource development basic plan for the stable supply of risk-managed water," the promotion of demand-led water resource development up to now has been changed to risk-managed. With the aim of shifting to a stable supply of water, the use of alternative water sources such as groundwater has been proposed as a flexible response in the event of a crisis.

On the other hand, since the quantitative impact assessment of the flow status of groundwater has been delayed, ground subsidence due to excessive pumping may occur due to improper regulation, on the contrary, it cannot be used effectively due to regulations.

Based on this situation, as one of the issues "Strengthening of National Resilience Against Natural Disasters" in the second phase of the Cross-ministerial Strategic Innovation Program (SIP) implemented by the Cabinet Office, "Integrated Study on Groundwater Utilization System at Water Outage/shortage during post-Disasters and/or Draughts" was adopted, and research began in 2018.

This system consists of "Development of social implementation interface" and "Integrated Watershed Model", and will be implemented and operated by the government, local governments and the basin council.

Multiple disaster scenarios are set in "Development of social implementation interface" to enable governments and local governments to understand the availability of water sources, including water demand and the water supply of surface water and groundwater as a whole in the affected areas, and to identify the amount and location of available groundwater.

In " Integrated Watershed Model ", we will develop a model that combines three advanced technologies: Integrated Watershed Model, New Forest Evapotranspration Model and Land Subsidence combined Watershed Hydrogeological Model.

Assuming the scenario set in the "social implementation interface" in the model area (Kanto Plain, Nobi Plain), the amount of groundwater that can be supplied is estimated under the standard of maintaining the land subsidence below a certain level.

In this presentation, we will introduce three advanced technologies and scenario analysis results.

Integrated Watershed Modelling for Groundwater Use at Emergency in the Kanto Plain, Japan

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Key Words: *Emergency use of groundwater, Watershed surface/subsurface coupled modelling, Hydrogeologic parameter identification, Groundwater potential*

For the purpose of mitigating water shortage/outage caused by possible natural disasters such as earthquakes or drought in the Kanto Plain which contains the Tokyo Metropolitan area of Japan, we have been working on numerical hydrologic modelling to investigate possibility of emergency water supply from groundwater wells.

For modelling the watershed which covers around 35,000km^2, a general-purpose hydrologic simulator GETFLOWS[1] was used, in which the interactions of the surface water and groundwater are treated in a fully coupled manner.

We collected necessary field data for numerical modelling as follows;

- DEM with 5m resolution
- Digital maps of vegetation and land use
- Hydrogeological information such as boring data, published maps and related bibliographies
- Records of surface/subsurface water use (location and rate with time)
- Climate records regarding precipitation distribution over the watershed
- Observation records of river flow (rate or water level), and groundwater level at wells.

The Kanto Plain is discretized with 250m horizontal resolution, and 60 variable thickness layers in subsurface down to -6500m. The final grid system was formed in around 46 million grid blocks.

For depicting the 3-D geological structure of the watershed, around 200 borings and other geological information/expertise were used to estimate geological structure of the whole watershed. Intensive calibration was made through comparison between the observed and calculated groundwater levels at over 100 wells, as well as the observed and calculated runoff rate for large rivers. The calibration processes were done by changing hydraulic parameters for the period of drought around 1994, and for the period from 1920 to present including the time when a large amount of groundwater was used for lives/industries from 1945 to 1970s.

In the presentation, we will introduce the tentatively obtained hydrogeological information such as

- Groundwater potential distribution (maps of permeability x thickness) ,
- Estimated cumulative thickness of muddy layers for estimating subsidence potential,
- Historical change of contours of groundwater level, and
- Flow lines from the past to the recent by graphics.

These hydrogeological information was transferred to the analysis of land subsidence.

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Integrated Watershed Modelling for Identifying Hydrogeological Condition and Groundwater Potential in the Nobi Plain, Japan

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Key Words: *Watershed Modeling, wide-area land subsidence, groundwater pumping, alluvial fan, unconfined aquifer.*

In the event of a disaster such as a large-scale earthquake, the function of water supply facilities may stop, and the water supply that is essential for people's lives may stop. The use of groundwater is effective as a water resource in such an emergency. On the other hand, unplanned use of groundwater may cause wide-area land subsidence and may cause various problems such as an increase in the risk of subsequent inundation.

We are constructing an integrated watershed model for identifying hydrogeological condition and groundwater potential in the Nobi Plain with the aim of quantitatively understanding when, where, and how much water can be pumped within the range that does not cause land subsidence. In constructing the watershed model, we keep in mind that 1) it is a model that matches the purpose, and 2) it is a model that captures the characteristics of the area related to the purpose.

The Pleistocene gravel layer distributed in the Nobi Plain is rich in groundwater recharged by the alluvial fan formed by the Kiso, Nagara, and Ibi rivers. In the Nobi Plain, which is rich in groundwater, wide-area land subsidence occurs due to the pumping of a large amount of groundwater during the period of high economic growth, and groundwater management including regulations is carried out to prevent this. As a result, wide-area land subsidence has subsided over time in recent years, but during the drought in 1994, although the annual pumping amount was below the control value, temporary groundwater pumping in the summer was progressed. As a result, ground subsidence has occurred. In an emergency such as a disaster, excessive pumping of groundwater may occur in the terms of time and space. This is considered to be exactly similar to the phenomenon of 1994.

In this report, we introduce that in order to construct a watershed model that satisfies the above requirements 1) and 2), we modeled an alluvial fan as a recharge source area, unconfined aquifer which is rich in groundwater and confining layer based on various information on topography and geology, and then simulated seasonal fluctuation trends in groundwater levels in 1994.

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Modeling of Line-Sources for Seepage Flow Analysis Allowing Arbitrary Finite Element Meshing

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Key Words: *finite element, seepage flow, line source, point source, unstructured grid*

A new model of line-source is proposed for the finite element method (FEM) of groundwater seepage flow. In the FEM, considering the pumping or injection (hereafter referred to as pumping) well, it is necessary to divide the pumping well and its vicinity into a very fine mesh to obtain accurate results. Because the diameter of the well is very small compared to the that of the analysis area, the well is often modeled as a line-source that is represented by a sequence of nodal points with given pressures or flow rates.

When modeling a pumping well with a sequence of point sources, each point source is considered as a well with a certain diameter according to the size of connecting-elements that connect to the point sources. Theoretically, the size of connecting-elements can be only approximately seven times the actual radius of the well, imposing significant restrictions on mesh division for large three-dimensional (3D) regions with planes of ten thousand of square meters or more.

Extensive research has been conducted earlier in the field of petroleum engineering to address this problem. Most of them are organized in the commemorative paper [1]. However, for 3D mesh, existing studies are only valid for the structured or the semi-structured grids. In this study, a new model of line-source for FEM accepting arbitrary 3D mesh is proposed to address this problem.

The proposed line-source allows the use of mesh that is divided by 3D finite elements of arbitrary shape. Because this model corrects only the permeability of the connecting-element based on the theoretical solution, its implementation into the existing programs involves creating only two subroutines. One corrects for permeability before constructing the FEM equations, and the other reversely corrects the velocity vectors and other factors related to the permeability after the solution. In addition, by making these subroutines as external programs, this model can be used as pre/post-processing of the existing programs or commercial software.

Analysis results of two simple problems are shown as code verifications for this line-source model after explaining the formulations and algorithm of the model in detail. One is the problem of a well pumping groundwater from the confined aquifer sandwiched between parallel impermeable layers, and the other is the problem of a well pumping groundwater from sections partitioned by packers for shielding groundwater. From these results, it was verified that the proposed line-source model provided considerably high accurate solutions even in arbitrary meshes.

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Scenario studies for safe use of groundwater during the post-disaster period

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Key Words: *groundwater, urgent usage, earthquake, drought, land subsidence*

Owing to the emergent situation under earthquake, flood and so on, the water outage is serious and grave damage to the suffers. Main countermeasure for water outages is emergency water-supply by a water tender. When the wide-area is damaged, the capacity of the water tender is not enough for water demand of suffers. Groundwater has the potential to support a part of water demand. On the other hand, groundwater intake has been limited to avoid land subsidence so far. Recently, the wise usage of groundwater for a risk-managed reliable supply of water is now considered. Here, we try to develop a scenario for the safe use of groundwater during the post-disaster period over the Kanto Plain including Tokyo, the capital of Japan, and Nobi Plain, including Nagoya, Japan. Those plains are at risk of earthquakes and drought.

The shortage of water resources was calculated as the amount of demand minus the supply. The amount of water outage after a disaster was estimated as the time series of water supply interruption rate based on past earthquake cases. This water supply interruption rate is high in areas at risk of liquefaction, where the risk of water pipe breakage is high, so the calculation was made separately from other regions. The demand for domestic water use was based on the demand for water for domestic use in each time series assumed in the disaster prevention plan by the Japanese government. Specifically, only drinking water (~3 liters per person per day) would be needed for the first three days after the earthquake, and that demand for washing and bathing (~250 liters per person per day) would increase as the days went by. These calculations were conducted for each municipality category and finally weighted and allocated regarding land use to create a 250m mesh of water shortage.

The developed scenario allows us to show the hot spots where the water demand is not met after the earthquake occurrence, depending on the season, climate condition, and distribution of seismic intensity of the earthquake. For example, in the downtown area, where urban development is not yet advanced, and wooden houses are densely built, there is a shortage of water to fight fires caused by earthquakes in many areas for the first day. In contrast, while outage of municipal water reaches its maximum around two weeks after the disaster event. The estimated time series of water outages at 250m mesh can be used as input data of the 3-D groundwater model to investigate the potential of groundwater safe of use without land subsidence.

Study of groundwater flow in Minami-soma City, Fukushima Prefecture, Japan

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Key Words: *Great East Japan earthquake, Groundwater Flow Simulation, Radioactive Cesium*

Due to the accident at TEPCO's Fukushima Dai-ichi Nuclear Power Station, radioactive materials were released over a wide area, and relatively high concentrations of radioactive cesium (hereinafter Cs) were deposited in the Abukuma Mountains. Although it has been clarified in previous studies that most Cs are strongly adsorbed on the surface soil, the possibility of Cs transport into the bedrock cannot be ignored in areas where the soil layer is relatively thin or where the basement granitic rocks are exposed at the surface.

Therefore, groundwater flow simulation with particle tracking analysis has been conducted in the area from the Abukuma Mountains (topographic high) to the lower coastal plain at the southern part of Minami-soma City, Fukushima Prefecture. The geological model has been constructed based on published topographical and geological information[1]. The geological model consists of Mesozoic granite in the west, Neogene sedimentary layers consisting of alternating beds of sandstone and mudstone in the east, and the NS-trend Futaba fault zone between them. The hydrogeological model was constructed by utilizing published hydraulic conductivity values[2] to geological zones of the geological model.

Regarding boundary conditions, constant head boundaries have been set for the side boundaries, while a no flow boundary has been set for the bottom boundary. Since actual measurements of hydraulic conductivity values are limited, sensitivity analysis has been conducted by changing the hydraulic conductivity of the Futaba faults zone and mudstone in the sedimentary formations.

As a result of the particle tracking analysis, most of the particles recharged from the mountainside discharge to three areas within a few years to several tens of years in the eastern plains regardless of differences in hydrogeological models. A groundwater reservoir exists within the discharge area above mentioned. This suggests that if Cs migrates with groundwater, Cs concentration may increase around the reservoir in near future. Therefore, it is important to conduct continuous monitoring of Cs concentrations around the reservoir.

A study on the effects of Cs in groundwater is expected to provide important information to citizens who are considering returning to this area.

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Uncertainty Analysis with Multiple Sets of Subsurface Properties for Land Subsidence Simulation using an Evolutionary Multimodal Optimization

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Key Words: *Land Subsidence, Inverse Modeling, Uncertainty, Evolutionary Multimodal Optimization*

This study tried an uncertainty analysis for numerical land subsidence modeling with multiple sets of subsurface properties which make comparable reproducibility of observed land subsidence by using an evolutionary algorithm for multimodal problems. Subsurface properties are often uncertain and multiple sets of subsurface properties can explain observed subsidence in numerical modeling, causing the reliability of a single "best" set to be questionable. Existing studies have attempted to solve this reliability problem through the ensemble Kalman filter or ensemble smoother, but these were not straightforward for highly nonlinear problems, such as a clay compaction process. It has also been reported that these methods can only deal with problems which have a small dimensionality in parameter space. This study aims to construct multiple sets by an inversion procedure of an evolutionary algorithm for the vertically 1D coupled simulator of groundwater flow and subsurface deformation with a modified Cam-clay model. The evolutionary algorithm has shown to be efficient and applicable for nonlinear problems, but it easily loses model diversity during the modeling process. We solved this problem by employing fitness sharing, which modifies the evaluation of a model according to its distance and similarity to neighboring models. As a result, we succeeded in obtaining diverse sets of subsurface properties with comparable reproducibility of observed land subsidence. Furthermore, the test of different thresholds for determining the size of the neighborhoods showed how the threshold controls the diversity of the obtained sets. Through an application to a synthetic problem, it was found that the hydraulic conductivity, specific storage, compression index, and the initial preconsolidation stress in clay and compression index in the aquifer are well-constrained, while the hydraulic conductivity and specific storage in the aquifer and initial void ratio in both clay and aquifer are uncertain. Finally, we demonstrate our method of visualizing the predictive uncertainty in land subsidence by applying it to an actual field problem and conducting the scenario analysis.

A Detailed Simulation Model to Evaluate the Crash Safety of a Li-Ion Pouch Battery Cell

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Key Words: *Electromobility, Crash Safety, Battery Modelling, Layered Cell Structure, Failure Analysis*

In crash situations with an electric vehicle, the integrity of the battery cells is critical for the consequences of the crash. A short circuit triggered by deformation and damage of the internal cell structure can cause overheating of the battery (thermal runaway) and may result in a vehicle fire or even an explosion. Thus, for assessing the crashworthiness of electric vehicles evaluating the deformation states of potential crash situations with respect to the occurrence of a short circuit is crucial. A particular challenge for building a cell model with acceptable computational time lies in the very different spatial scales regarding the overall cell size and the thickness of individual layers. Cells installed in vehicles have dimensions of several centimetres, whereas the thickness of the individual layers is in the micrometre range. Much research has already been conducted based on homogenized cell models that do not explicitly account for the internal layer structure, and existing material models calibrated to experimental data (e.g. [1]-[3]), while explicitly considering the layered structure is just pursued more recently (e.g. [4]-[7]).

Within our contribution we introduce a detailed numerical model which, as a part of a multilevel simulation approach, can be used to evaluate the criticality of a deformation state. The model mimics the layered structure of the cell, whereby the constitutive properties were determined by in-house experiments on the respective materials. For validation, bending tests and indentation tests with different punch geometries along with CT-scans at selected indentation depths are available. Comparing the simulation results with the failure sequence and the force-displacement curve from the experiment, a closer view on critical deformations and on their respective stress states is obtained. The results indicate that in-depth understanding and modelling of the failure behaviour is crucial for correctly modelling battery cells under crash loading scenarios.

Acknowledgments

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15th World Congress on Computational Mechanics (WCCM-XV)
8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII)
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Application of the CAE/ML technique for coupling analysis between vehicle structure and occupant safety

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Key Words: *Machine Learning, Multi-disciplinary Optimization, Crash Simulations, Occupant Safety Simulations*

In the early stage of vehicle planning phase, feasible designs based on the vehicle plan should be derived to meet the lower development cost and working hours.
Conventional finite element analysis from CAD drawings can't find the feasible area in the design space without long hours of CPU.

To conduct feasibility study in the early stages of vehicle planning phase for vehicle body deformation and occupant safety, the database was constructed from large number of frontal crash FE analysis using parametric FE models.

Machine learning(ML) models were created from the database. Coupling analysis using ML models between vehicle body deformation and occupant safety enables occupant injury value predictions from design variables for the vehicle body frames.

Artificial Intelligence with Dimension Reduction Methods for Applications in Shape Recognition

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Key Words: *3D-objects, 1D-like Features, Artificial Intelligence, Automatic Shape Recognition, Mesh Generation*

In recent years, a wide range of different approaches have been proposed as shape recognition techniques for 3D objects. The important key for efficient and practical operation in real world is proper engineering of the data representation [1-2]. Vast majority of data representation for 3D objects is based on image-processing methods. Meanwhile, the algorithm to effectively extract data representation (high-level representation) from the raw 3D data is still under study. In this paper, an attempt to define high-level representation is proposed, where the raw 3D data can be extracted into a simplified 1D-like data. Besides data simplification and dimension reduction, the experimental results show no significant loss of accuracy. This 1D-like data is then used as an input into machine-learning system to be manipulated for shape recognition.

3D objects are basically made up of multiple surfaces that can be split separately. Here, data representation of each surface is calculated using our proposed methods to obtain 1D-like features information [3]. The extraction of 1D-like data from surface properties is proposed in [4], which consists of geometrical descriptors, face angle, point angle, etc. Therefore the real 3D objects can be simply modeled as 1D-like data arrays collected from the overall surfaces. This method is able to construct data representation with less computation power and time respectively.

An experiment was carried out to evaluate the performance of dimension reduction methods implemented in machine learning (deep-learning algorithms) for use in 3D shape recognition with a task to predict the label for each surface. The proposed method has achieved satisfactory result with accuracy > 90%. The advantage of this proposed method is the computation speed of data extration, which makes it attractive as a potential candidate for high-speed shape recognition in real practice. Further works are under going to improve the recognition accuracy and robustness.

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Generation of abuse simulation models of battery cells and battery packs

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Key Words: Multi-phyiscal Model, Battery Cell and Pack, Abuse Testing and Simulation

In accordance to several safety requirements, battery packs have to pass certain tests defined by international standards and regulations. Particularly, the avoidance of the effect of thermal propagation, induced by a single cell and resulting in a catastrophic failure of the whole pack, has to be addressed within the design process. Aiming for an efficient optimization of the overall safety behavior, multi-physical models of the battery pack as well as of the applied battery cells are required. This contribution introduces a standardized and automatable generation methodology of the required simulation models. Aiming for the initial characterization of the single battery cell, specific experimental investigations are performed. In addition to an electrical and thermal characterization, electrical as well as thermal abuse tests are carried out. Based on the experimental results, the relevant model parameters are identified. To this end, specific multi-physical models are created and evaluated in the commercial finite element code LS DYNA. Here, a self-developed tool is utilized, which allows for the automatic generation of these models. Note, that various modeling approaches ranging from homogenized scale models down to layer level models can be considered with respect to the desired discretization. To validate the resulting model of a single battery cell, some tests are exemplary simulated and the results are compared to the experimental data. In addition, the arise of the thermal runaway is analyzed with respect to the location of the initial short circuit and the state of charge. Next, a model of one investigated battery cell is integrated in an abuse simulation of a whole battery pack. Finally, the simulation results allow for a study and discussion of the influence of specific design measures on the avoidance of thermal propagation. Consequently, the full range from experimental characterization and abuse testing of single battery cells to abuse simulation of whole battery packs is covered by this contribution.

Investigation of Internal Deformation of Lithium-ion Battery and Simulation Model for Internal Short Circuit

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Key Words: *Lithium-ion battery, Internal short circuit, Digital microscope, SEM image, Shear band, FEM, DEM, Simulation, Ansys LS-DYNA*

A fire accident caused by the thermal runaway of the Lithium Ion Batteries is one of the important issues of practical electric vehicles. As a safety testing for electric vehicle, thermal runaway and white smoke generation due to impact and crush tests is often evaluated. Basically, though the short-circuit is considered to be caused by the contact between the positive and negative electrodes[1], it is difficult to confirm what kind of deformation occurs inside the battery, because the battery explodes by a short circuit and thermal runaway. The purpose of this research is to elucidate the mechanism of the internal short circuit by visualize the internal deformation state when an internal short circuit occurs. First of all, in order to investigate the inside of Lithium Ion battery during large deformation, the battery was held and solidified in its deformed state, and the internal deformation is observed by digital microscope. In according to the observation in section plane of deformation state, the aluminum and copper of the current collector foil were broken in the upper layer. Furthemore, a shear band could be confirmed by connecting the points of the broken collector foil. It is presumed that this internal deformation state is the cause of the contact between the active materials of the positive and negative electrodes and the contact with the foil, which causes an internal short circuit. This result is important to explain why battery cells cause internal short circuits when large deformation has occurred. In addition, in order to elucidate the mechanism of this shear band, we will introduce a proposal to elucidate the internal short-circuit generation mechanism by constructing a simulation model that can reproduce the shear band by compression by using the commercial finite element method code Ansys LS-DYNA.

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Simulation of Stretching Deformation of Films for Electronic Devices in Automotive Applications

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Key Words: *Finite Element Method, Orthogonal Anisotropic Plasticity, Fluoropolymer, Film, Biaxial Stretching, Transverse Stretching, Deformation, Kink Band*

Fluoropolymers have excellent weather resistance, heat resistance, electrical insulation properties, etc., and are used in a wide range of fields such as semicondutcors and automobiles [1]. Recently, it has been clarified that the electrical properties such as relative permittivity, volume resistivity and dielectric breakdown strength of the fluoropolymers are significantly improved by controlling their crystal structure with biaxial stretching [2]. As a result, biaxially stretched fluorine films are increasingly expected to be used in automobile-related electronic devices such as high-frequency substrate films, motor insulating papers, and film capacitors to improve their performances and reduce their sizes and weights. For example, the size of the film capacitors can be reduced to less than half with the fluorine films compared to polypropylene (PP) films. As automobiles become CASE (Connectivity, Autonomous, Sharing/Subscription, Electrification), various devices are required to be smaller and lighter. The downsizing of the film capacitors will greatly contribute to the miniaturization and performance improvement of the electronic devices for electric vehicles. However, it is difficult to continuously manufacture the fluorine films because kink bands and stretching tears are easily to occur during successive biaxial stretching with a tenter.

In this study, we proposed a simulation method for film transverse stretching based on the finite element method using the orthogonal anisotropy plastic model [3]. The simulation method can not only analyse the large stretching deformation up to the orientation hardening region, but also predict the kink band phenomenon that occurs during the film transverse stretching. The validity of the simulation method was confirmed by the film transverse stretching tests performed on the fluorine film sheets with different longitudinal stretching ratios. Using the simulation method, we clarified that the anisotropy index of the fluorine film sheets has a great influence on the presence or absence of the kink band phenomenon during the film transverse stretching. The anisotropy index of the film sheets after longitudinal stretching can be related to their orientation, and the two are approximately in a linear relationship for the fluorine film sheets. Moreover, we revealed the change in film stretching deformation due to difference in tenter shape. The main conclusions drawn by the simulations are as follows.

(1) The presence or absence of the kink band phenomenon during transverse stretching largely depends on the anisotropy of the film sheets after longitudinal stretching.
(2) The ratio of length to width of the stretching zone is desired to be 2.0 or more.
(3) The protective layer attached to the edge of the film sheet has the effect of preventing the film from tearing during the transverse stretching.

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The UPSCALE project. Physics informed machine learning turbulence modelling applied to vehicle aerodynamics

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Key Words: *CFD, PIML, turbulence modelling, aerodynamics, machine learning*

The UPSCALE project is the first EU funded project intended to integrate Machine Learning (ML) algorithms with CAE tools to foster the development of Electric Vehicles. Within the frame of the UPSCALE project several innovative solutions that apply this premise have been implemented and tested on real vehicle designs. Examples of this new approach to simulate key automotive load-cases include surrogate models of aerodynamic CFD simulations, reduced order models of battery cells in crash simulations or machine learning physics informed (PIML) turbulence models.

In this work, we present the application of machine learning to find a correlation between Reynolds (Re) stresses and the main flow variables in high fidelity flow fields, with the aim to set an iterative process to progress through RANS solutions with realistic flowfields including, pressure, velocity and Re stresses.

Following the approach proposed by *Xiao* [1],the authors implemented a framework that extracts up to 10 variables (inputs in our ML model) and 8 responses (outputs ion our ML model) in RANS and DNS flowfields and tried different strategies to improve the RANS solution accuracy and trying to be closer to DNS flowfield.

Framework 1 is focussed on computing the discrepancy between RANS Re stresses and the would be Re stresses in the DNS solution. So, we use RANS flowfield variables as inputs and the difference between RANS and DNS Re stresses as output to train the ML algorithm. This approach proved to be promising for similar flowfield, with same geometry and Re number, showing its limitations when moving to complete different flowfields**.**

In framework 2, we use high fidelity data only as inputs and the DNS Re stresses as outputs for the training phase and we apply this rule on the RANS inputs to get a new Re stress field. The direct application of this approach on converged RANS flow-fields proved to be unsatisfactory, and the authors deem this is due to inaccuracy of the converged flowfield, so further investigation needs to be performed, for instance a coupled procedure between the Navier Stokes equations solver and the PIML Re computation.

The presentation will include the description of the different investigated frameworks, the main results, conclusions and the foresight of the application Physics informed strategies in turbulence modelling.

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Credible, Automated Meshing of Images

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Key Words: *Image-based simulation, uncertainty quantification*

Image-based simulations are a key enabler of digital twins and can represent a digital engineering workflow for the analysis of as-built materials and components. In this talk, we detail the development of key enabler technologies for credible and automated image-based simulation workflows. Machine learning techniques are created for 3D image segmentation with uncertainty, which we show to be more robust and accurate than human segmentations. We also extend the conformal decomposition finite element method to automatically generate high quality meshes for numerical simulation. This entire workflow is subjected to rigorous uncertainty quantification. Our processes are demonstrated on three key exemplar applications, thermal protection system materials, electrodes for lithium-ion batteries, and exploding bridge wire detonators.

Additionally, we have fully automated this image-based simulation workflow with a cloud-computing-based web interface. We demonstrate this automation on the exploding bridge wire detonator exemplar.

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Deformation Analysis of Realistic Structure Using Virtually Laser-Scanned Point Cloud on Partial Surface

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Key Words: *Nonlinear Finite Element Analysis, Deformation Analysis, Point Cloud, Laser Scanning*

Abstract

In recent years, with the advancement of technology in shape measurement and geometry processing of structures using terrestrial laser scanners (TLS), it becomes possible to create finite element analysis models from the point cloud measured by TLS.[1,2] In the methods presented in the previous studies, the shape of the structure at the time of point cloud measurement is used to generate the analysis model before deformation. However, the actual structure is already deformed at the time of point cloud measurement even when it was constructed just the moment. The existing studies ignore the deformation until the shape is measured.

To perform structural analysis including deformation before measurement, an analysis method that considers the point cloud data as a deformed partial shape of the structure was proposed in this study. In this method, it is assumed that drawings or CAD data of the structure exist. The deformation analysis is performed so that the finite element analysis model obtained from these data matches the partial point cloud data after deformation.

Beams, which are basic structural mechanics problems, were analyzed to investigate the performance of the proposed method. Point cloud data created virtually were used in these analyses before applying this method to real structures. In the presentation, we will present a numerical analysis of a more complex and realistic structure by using point cloud data.

Acknowledgment

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Co-Creative Design of Adhesives of Multi-materials by Shape Optimization under Multiaxial Stress Failure Criteria

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Key Words: *Co-creative design; Adhesive; Shape optimization; Failure criterion; Multiaxial stress state*

An important technical trend in the automotive industry in recent years has been a reduction in the weight of structures in an effort to reduce the emission of carbon dioxide and energy consumption. One strategy adopted to lighten structures is multi-material design. [1] Among various methods of joining dissimilar materials, adhesive bonding has the advantage of being low weight. The problem of adhesive bonding is complicated that both material factors and structural factors affect the strength and design process. As a result, a co-creative design process is necessary to involve all those factors into the application of adhesive bonding.

For material factors, experiments using pipe specimens with inclined surfaces bonded by epoxy adhesive were performed, whereby multiaxial stress states were realized simply by conducting a uniaxial tensile test. The failure function of the epoxy adhesive, expressed by the mean stress and octahedral shear stress, was then obtained from the experimental data and compared with that of acrylic adhesive previously reported in the literature. [2] For material factors, the obtained failure functions of both adhesives were then applied to the shape optimization of the adhesive layer under different loading conditions. The optimization object is the strengthening of jointed structures. The optimal shape for different loading conditions differed for the different adhesives because of the driving force generated by the applied stress. [3]

The final shapes were thus optimized numerically and found to be strongly dependent on the initial shapes before optimization. We found that these final shapes are numerically optimized to realize a higher mechanical integrity of the adhesive layer. The patterns of the shape changes during the optimization process differed according to different loading condition as well as different adhesives which could be indicated by the shape gradient function inducing the geometric change of the adhesive layer. The research is expected to provide a procedure of co-creative design of multi-materials using adhesives. The observation of the shape optimization could be used as an indicator of whether the initial model is appropriate for multi-material design.

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Elastic-Plastic Constitutive Law of Deformation History Integral Type for Rubber Material of High-Damping Rubber Bearings

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Key Words: *Seismically isolated structure, High-damping rubber bearing, Finite element analysis, Elastic-plastic constitutive law*

New elastic-plastic constitutive law for rubber material of high-damping rubber bearing was developed. High-damping rubber bearing is one of the seismic isolation bearings which are important members of seismically isolated structure. In design of the seismic isolation bearings, finite element analysis (FEA) is widely used as a method of numerical simulation. Generally, in design of rubber-like material based on FEA, selection of a constitutive law is particularly important. There are many types of seismic isolation bearings, however, high-damping rubber bearing shows complex behaviour compared with other seismic isolation devices. It is one of the feature of rubber bearing that magnitude of deformation is much larger than other rubber products and the maximum shear strain of rubber is about 400%. In the past, many constitutive laws for FEA of high-damping rubber were proposed. However, they could not represent the complex behavior of restoring force characteristics of high-damping rubber bearing with high accuracy. Thus, authors developed new elastic-plastic constitutive law for rubber material of high-damping rubber bearing. The constitutive law is called deformation history integral type model (DHI model). The model was developed as elastic-plastic constitutive law by modifying Simo's viscoelastic constitutive law [1]. The model is defined by the relationship between second Piola-Kirchhoff stress and right Cauchy Green tensor. Features of proposed constitutive law are as follows;

A. DHI model can represent the horizontal creep behavior when strong wind such as hurricane, cyclone and typhoon hits seismically isolated structure using high-damping rubber bearings.
B. DHI model can represent the complex behavior of high-damping rubber bearing for wide range of shear strain including horizontal bi-directional loading.
C. Calculation algorithm of DHI model is very simple and calculation cost is low.

Accuracy of the proposed constitutive law was confirmed by comparing various test result of high-damping rubber bearing. While new constitutive law was developed for high-damping rubber bearings, the model has the potential to apply to other materials and products.

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Homogeneous Finite Element Analysis of Polyurethane Foams using Kelvin Unit Cell

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Key Words: *Homogeneous finite element analysis, Kelvin unit cell, Polyurethane foam*

In this study, the homogeneous finite element analysis using the Kelvin unit cells was performed to evaluate the macroscopic mechanical properties of the polyurethane foams considering their microscopic structures.

The mechanical properties of foam materials have been evaluated by the homogeneous finite element analysis with unit cells [1][2]. The unit cells were required to represent the geometric feature of the microscopic structure from the engineering point of view.

The Kelvin unit cell was introduced to represent the microscopic structure of the polyurethane foams. In this study, the Kelvin unit cell consisting of 6 squares and 8 hexagons was applied to the numerical simulation. There are 36 beams and 24 edges in one unit-cell. Three-dimensional CT scanning images were observed to create the Kelvin unit cell considering the microstructure of the polyurethane foams. The beams of the polyurethane foams have a non-uniform distribution of cross-sectional areas along their length. The non-uniformity of beam cross-sectional areas was given to the Kelvin unit cell to reproduce the microstructural geometry of the polyurethane foams.

The hyperelastic material was applied to the matrix of the Kelvin unit cell. The higher order Yeoh model was adopted to the potential energy function of the hyperelastic material. The original homogeneous finite element analysis code of the Kelvin unit cell was developed. The mechanical properties of the polyurethane foams in the uniaxial compressive deformation were evaluated by the analysis code. From the analysis, the non-uniformity of beam cross-sectional areas is an important factor for the mechanical properties of the polyurethane foams.

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Implementation of the hyperelastic, hyperelastic plus damage, and hyperelastic plus viscoelastic models in the UMMDr subroutine library

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Key Words: *UMMDr, hyperelastic, damage, viscoelastic*

With the diffusion of commercial finite element software, practical problems have been solved by numerical simulations in a wide range of fields. However, for more advanced problems, we require material models that are not prepared using the default analysis options. For this reason, computer aided engineering (CAE) engineers need to customize the options available in finite element programs themselves and consider the material model appropriate for the problem, but these technical processes require specialized knowledge and skills.

The Japan Association for Nonlinear Computer Aided Engineering (JANCAE)[1] offers information and learning opportunities to CAE engineers in various positions. Since 2011, participants have developed and verified two user subroutine libraries: the Unified Material Model Driver for Plasticity (UMMDp) for anisotropic yield functions, and the Unified Material Model Driver for Rubber (UMMDr) for modeling rubber materials. We announced the release of the UMMDp[2] at the 2018 WCCM, and will announce the UMMDr this year.

In the UMMDr, a subroutine library combines the hyperelastic models (e.g., stretch-based models such as Ogden and Shariff, and invariants-based models such as Mooney Rivlin.), damage models (e.g., Simo, Miehe, Ogden-Roxburgh[3]), and visco-elastic models (e.g., Simo, Holzapfel,[4] Reese-Govindjee[5]). Using these models, the stress and consistent tangent stiffness for a given deformation gradient are calculated, and converted to the stress rate or the alternative stress that is suitable for each commercial finite element software, such as Abaqus, ADINA, Ansys, Ansys LS-DYNA, Marc, and Simcenter Nastran. Therefore, new constitutive models can be added to the UMMDr just by creating a new subroutine.

In this presentation, we will explain the structure of the UMMDr and how to introduce a hyperelastic model, a damage model, and a viscoelastic model into the UMMDr. We will also demonstrate verification using some simple tests.

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Multi-Scale Simulation of Filled Rubber Composite with Molecular Dynamics and Large Scale FEM Analyses

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Key Words: *Multi-scale analysis, Filled rubber, Molecular dynamics, Finite Element Method, the K computer*

In order to establish a sustainable society, superior rubber materials for tires are required so that both the rolling resistance and wear performance can be improved. It is known that visco-elastic characteristics of rubber material plays an important role for these performances. Filled rubber is a nano-scale composite made of matrix polymer such as natural or synthetic rubber, and filler particles such as carbon black or silica. Precise study in mechanical behaviour of matrix polymer, filler particles, and their interactions is expected to explore the origin of visco-elastic properties. However, it is very difficult to do it by experiments.

This study aims to develop a simulation technology which can predict the visco-elastic response of nano-composite by numerical simulations. A multi-scale computational modelling method is proposed. Both molecular dynamics (MD) and large scale Finite Element Method (FEM) are utilized to include molecular level properties into continuum level analyses. MD resolves the matrix-filler interaction in the molecular scale to obtain the thickness of the interphase region and the mobility of molecules of the matrix polymer within the region. These results are passed to the FEM analyses where nano-scale filler structures are precisely modelled from the images measured by 3-dimensional transmission electron microscope tomography (3D-TEMT). The FEM computations are done by 6144 cores of the K computer since the numerical model becomes around 200 Million degree of freedoms.

The effects of filler-matrix interaction intensity and filler dispersion are analysed, and the differences in relaxation modulus are presented to show the effectiveness of the proposed method.

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Practical examples using Unified Material Model Driver for Rubber

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Key Words: *UMMDr, rubber, damage, finite viscoelasticity*

The Japan Association for Nonlinear Computer Aided Engineering (JANCAE)[1] provides information and learning opportunities for CAE engineers in various positions. As part of the activities of the subcommittee for non-linear material modeling, since 2011 we have been developing a material model driver, the Unified Material Model Driver for Rubber (UMMDr), to handle the constitutive laws of rubber like materials in a unified manner. The model consists of a hyperelasticity branch with damage and finite strain viscoelasticity branches in parallel. The user selects hyperelastic models, such as Ogden, Mooney-Rivlin and Extended-tube,[2] and can also select damage models, such as Ogden-Roxburgh,[3] or finite strain viscoelastic models, such as Holzapfel[4] and Reese.[5] It is possible to consider the damage model and the viscoelastic model at the same time. One can also add their own new constitutive model to the UMMDr.

In this presentation, we report on two practical examples of using the UMMDr in the following codes: Abaqus, ADINA, Ansys, Ansys LS-DYNA, Marc, and Simcenter Nastran (with Samcef Mecano as the solver behind the solution). In the first example, we evaluate hyperelastic-viscoelastic properties by repeatedly performing simple shear deformation of a cube. In the second example, we evaluate hyperelastic-viscoelastic properties by repeatedly performing compression of a rubber bushing. Normal outputs were obtained for each code.

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Spectral Analysis on Surface Roughness in the Initial Wear Process of Tire Rubber and its Modeling

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Key Words: *Tire rubber, Friction, Wear, Surface roughness, Power spectral density*

A full understanding of the wear phenomenon of frictional tire rubber on a road surface plays an important role at predicting the tire life with high accuracy. Although the multiple analyses including adhesion, hysteresis and ploughing friction may be required for elucidating the wear mechanism, such a comprehensive analysis needs a high-cost performance because various contact and fiction mechanics at the corresponding scales should be implemented. Therefore, the present tire-life prediction is to use the stationary equation of wear volume, estimated by tire wear tests with a belt-type or drum-type machine. It is not efficient in the terms of intensifying the development cycle of a tire.

In this study, we focus on the initial wear process of tire rubber, in which the abrasive wear severely proceeds along with the change in a statistical nature of surface topography. We demonstrated the reciprocating friction tests with carbon black-filled rubber specimens and a vitrified grindstone plate. Measuring the pre- and post-sliding surfaces of the rubber specimens, we carried out the spectral analysis on the measured surface height data to compare with that of the grindstone substrate using a correction method of the areal 2D power spectral densities (PSDs) [1]. To convert the 2D PSDs to the isotropic PSDs and fitting them with the K-correlation model [2, 3], we revealed that the average Hurst exponent (H) of the rubber surfaces approaches asymptotically to that of the substrate with the increase of sliding distance (d). We also calculated the relative wear volume (V_{rel}) using H within the high wavenumber range and clarified that the curve of $V_{\mathrm{rel}}(d)$ can be expressed by the logistic equation, which is the model of population growth in the field of ecology. Our findings open the elemental wear mechanism of soft matter on a rough and hard substrate, which could link to the stationary wear process of our practical interest.

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Study on Evaluation of Viscoelastic Hyperelastic Properties of Polymer Foam Materials Using Voxel Finite Element Analysis

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Key Words: *Polymer foam, Microstructure, Voxel FEM, Microscopic CT-scan*

In this study, voxel finite element analysis(FEA) of microscopic structure of polymer foam were performed to reproduce its viscoelastic behavior.

Finite element models were created from 3-dimentional microscopic CT-scan data of the polymer foam material. A polyurethane foam for automobile seats was applied to the polymer foam in this study. The tensile loading test specimens of polymer matrix without air-bubbles were created by original defoaming-process. The viscoelastic properties were obtained from tensile loading test results of polyurethane matrix.

Viscoelastic hyperelastic model was applied to reproduce the stress-strain relationships of the polymer-matrix. The polyurethane-matrix was confirmed as nonlinear elastic and weak viscous material. Compression loading tests of the polymer foam materials were conducted under some relative density. The effect of relative density on the mechanical properties was evaluated by the loading test results.

Effects of microstructure were simulated by the voxel FE analysis with 3-dimentional microscopic CT-scan data. The analysis results were compared with stress-strain relationships obtained from compression tests of the polymer foam materials.

Three-FE models were applied to the voxel FE analysis. The number of elements in each models was 1,194, 1,254, and 1,263, respectively. Effect of microstructure on the macroscopic mechanical behavior of foam material were appeared in plateau-area. Location of stress concentration in microstructure of the foam materials was shown to be consistent at different strain rates by the simulation results. Viscous effect of the polymer matrix on the macroscopic mechanical behavior of foam material were shown in the simulation results.

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An efficient CFD model of an industrial scale CVD reactor allowing accurate coating thickness predictions

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Key Words: *Chemical Vapor Deposition, Computational Fluid Dynamics, Alumina deposition, Industrial-scale Reactor*

This work presents a two-dimensional, time-dependent, computational fluid dynamics (CFD) model of an industrial-scale Chemical Vapor Deposition (CVD) reactor, used for the coating of cutting tool inserts. In CVD processes, a gas reactant mixture enters the reactor chamber and through a series of homogeneous and surface reactions, leads to the deposition of a thin film on a heated surface. The developed CFD model accounts for the transport of mass, momentum, and chemical species inside the reactor while including a simple reaction scheme for the deposition of alumina.

The reactor used for the production of the alumina coatings consists of around 45 perforated trays, stacked one on top of the other. The cutting tool inserts are placed on each tray on appropriately sized structures. The gas reactants enter through perforations which are carefully placed on a central rotating tube. This ensures the uniform distribution of the gas reactants around the inserts. The simulations aim to capture the effect of the gas flow field on the coating thickness and, in extension, on the coating thickness uniformity. Providing accurate thickness predictions will enable the implementation of the model as an optimization tool for the production setup. However, implementing such a model in everyday production is not feasible unless the model is efficient in terms of the required computational resources. This consecutively leads to several challenges, such as simplifying the three-dimensional geometry coupled with the physically meaningful incorporation of the rotating gas feed tube in the model.

The model's predictions are compared with α-Al_2O_3 coating thickness measurements available for different locations inside the reactor. The model can accurately predict the coating thickness with an average relative error of 5%. The model allows for simulations of several different reactor configurations and process parameters and can therefore be used to study the effect of these factors on the resulting coating thickness.

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Development of a hybrid model for large-scale plant RUL prediction based on data and physical models

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Key Words: *Predictive maintenance, Machine Learning, Industrial Applications, Optimizing maintenance intervals, Remaining Useful Life*

Large plants in the process industry are monitored and maintained at regular intervals, and repeatedly maintenance is either too early or too late. This causes unnecessary costs due to technicians, spare parts procurement as well as delivery issues and to high downtime costs due to unexpected shutdowns. In this context, the Remaining Useful Life (RUL) plays a major role, as it is an indicator of how long a machine or component can run without breakdown, repair or replacement. By predicting RUL using predictive maintenance, maintenance can be better planned, operational efficiency optimized, and unplanned downtime avoided. Optimizing the prediction accuracy should therefore always be in the foreground and is therefore the topic of this abstract.

Lei et al. [1], in a review on data acquisition to RUL prediction, emphasize that predicting the operational behavior of machinery and equipment is one of the major challenges in condition-based maintenance. According to the authors, such a prediction program consists of the following four technical processes: 1. data acquisition; 2. construction of the Health Indicator (HI) of machinery and equipment; 3. subdivision into different stages of the Health Stage (HS); and 4. RUL prediction. The relevance of RUL prediction is also supported by Jimenez-Cortadi et al. [2]. Analogous to Lei et al. [1], Jimenez-Cortadi et al. [2] list different approaches and techniques, but the main contribution is finding a solution to the prediction problem in real machine processes. The results show that preventive maintenance can be transformed into predictive maintenance. In this context, the goal of predictive maintenance is to extend the life of machines and equipment. Jimenez-Cortadi et al. [2] used a CNC milling machine as a real example and used machine-learning techniques to predict the RUL. However, the authors emphasize that the complexity of the model made it difficult to implement in the production machine. Another approach would be a hybrid modeling; this is also emphasized by the authors in Arias Chao et. al [3]. To combine the advantages of both models physical and data-driven, which on the one hand draws on the information of physical models and on the other hand uses deep learning algorithms. The results from the experiment [3] show that the hybrid model outperforms purely data-driven models in terms of predictive power - the prediction horizon could be extended by about 127%.

The hybrid model is enhanced by the physical model to evaluate and prioritize the wear of the plant condition under the given operating conditions and influences. The hybrid model is applied to a real process gas industry. The basic questions are: What was defective and what was repaired? Which components fail most frequently? Which components have to be replaced or repaired at high cost? The prerequisite for this is service and repair data. The physical model describes a functional relationship between operational stress and service life. The remaining service life is finally predicted by determining whether and when the predicted parameters meet the failure criteria from the failure description. The task is to elaborate the technically essential aspects from the point of view of the modeling of mechanical components under the consideration of dynamic quantities and simulation of a large industrial plant. The goal is to correlate the anomalies found by the hybrid model as well as possible with future faults. Such a trained model can be of great importance for industrial real-time applications; after all, the anomalies identified by the model can enable predictive maintenance for complex large-scale plants.

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Improving prediction of wind loads on buildings using machine learning

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Key Words: *Wind loading, Machine learning, Computational fluid dynamics, RANS, LES*

Computation fluid dynamics (CFD) represents an attractive possibility to be used for the design of structures. Nevertheless, routine use of the CFD for design purposes still requires significant progress to guarantee the right balance between accuracy of the results and computational efficiency [1].

On the one hand, Reynolds-averaged Navier-Stokes (RANS) simulations are widely employed in wind engineering applications due to their low computational cost. However, their inability to accurately predict complex features of the flow, such as separation and reattachment is limiting their application to qualitative analysis [2, 3]. Thus, RANS-based calculation of the wind loads is generally considered as insufficiently accurate [1], as it is even challenging to obtain a quantitatively accurate prediction of the mean pressure field. On the other hand, Large Eddy Simulation (LES) can provide more accurate prediction of wind loads, but with significantly higher computational costs. In this specific case, wind loads on the the building, these computational costs are even more emphasized as different wind directions of approaching flow needs to be considered.

Therefore, the aim of this study is to propose an optimal machine learning framework that combines computationally efficient RANS, for several wind directions, with more expensive LES for fewer wind directions to provide accurate predictions and lower the computational cost. The developed model takes the RANS mean flow variables, such as mean pressures, coordinates, angle of attack and others as an input and predicts LES obtained mean and rms pressure coefficients. Those LES results are validated with the wind tunnel results. Feature selection techniques are used to explore the optimal combination in terms of accuracy, but as well to reduce the computational cost of modelling. Different machine learning algorithms such as support vector machine, gradient boosting, random forest, and artificial neural networks are adopted and hyperparameter optimization is done to increase the accuracy. Optimal set-up for each of the output parameters, mean and rms pressure coefficient on the building surfaces is presented.

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Optimizing the Energetic Efficiency in Autonomous Underwater Vehicle (AUV) Group by A Multi-Level Computational Model

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Key Words: *Computational Fluid Dynamics, Autonomous Underwater Vehicle (AUV), energy-saving formation, multi-level CFD, optimization, engineering application, potential flow*

Swimming and flying animals can improve their energetic efficiency by moving through fluids in formation (e.g. [1]). It is reasonable to expect that Autonomous Underwater Vehicle (AUV) Group may also adopt specific formation to optimize energetic efficiency, which may significantly benefit our future AUV-group-based exploration, development, and cleaning in ocean.

This challenging hydrodynamic problem is solved by a multi-level numerical approach, which consists of individual- and group-level solutions.

The individual-level simulation provides accurate propellor power at cruising speed, the gradient of power with respect to speed around cruising condition, as well as the flow field around the AUV. We modelled a full scale AUV, and perform simulation by commercial software STAR-CCM+ (SIEMENS, Germany [2]) with Reynolds averaged Navier-Stokes (RANS) turbulence model. The result is then input as source information for the group-level solution. Unsteady flow field is time-averaged into a steady axisymmetric flow.

The group-level simulation is based on an analytical potential-flow model, we approximate the velocity field far from an individual AUV by the velocity field of a vortex ring and a momentumless wake. This allows us to investigate equilibrium formations for groups of AUVs and evaluate the perspective of energy saving through their far-field interference.

By solving the flow system that consists of the superposed elements and constraints set on the relative position of the AUVs, we formulate an optimization problem for minimizing the power at a given speed, and find optimal formations using numerical methods of global optimization. Our result reveals optimal formation formed by several to tens of AUVs.

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A Comparison Study between Isogeometric Analysis and Finite Element Analysis for Nonlinear Inelastic Dynamic Problems with Geomiso DNL Software

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Key Words: *Isogeometric analysis, Finite element analysis, Computational structural dynamics, Inelastic analysis, T-splines, NURBS, Accuracy, Convergence, Computational cost, Cloud*

This research aims to compare the efficiency of isogeometric analysis and finite element analysis for nonlinear inelastic dynamic applications with the recently developed Geomiso DNL program. Geomiso DNL is a hybrid software solution, which combines isogeometric analysis and 3D design with NURBS and T-splines. The isogeometric method satisfies the rising industrial need for unification of the fields of computer-aided design and computer-aided analysis, while modern T-splines overcome limitations inherent to NURBS, permit local refinement, ensure higher-order continuity across patches, and provide great superiority of modeling irregular geometries with hole features. Therefore, this powerful generalization of the classical finite element method has attracted growing interest in both scientific community and industry.

Geomiso DNL is not just a plug-in, but a both on-premises and cloud-based software, which enables engineers to simulate dynamic phenomena, whose impact on products and structures in real-world environments can be more efficiently evaluated. This new software fully integrates the industrial design of any geometry with its computational real-time testing by facilitating the geometry modeling within analysis. A key feature is that this hybrid program provides parameterized geometries in the design, as it weaves the mesh generation process within CAD, while its comprehensible modern graphical user interface offers an innovative way to preserve the exact geometry at all refinement levels in contrast with finite element programs.

Applications to nonlinear plane stress, plain strain, and three-dimensional dynamic problems are demonstrated with a comparison between Geomiso DNL and finite element software packages. We compare the matrix assembly and solver time, as well as the accuracy of the numerical results, such as displacement, strain and stress fields, for typical examples arisen in structural dynamics. We also perform parametric tests on the effects of polynomial order of shape functions and the number of patches, elements, control points, and quadrature points. This program appears to be preferable to finite element software packages, as it represents major improvements, such as higher accuracy, robustness, and stability level, combined with significantly shortened computational cost. This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call «RESEARCH–CREATE–INNOVATE» (project code: T2EDK-00338).

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An Alternative Approach for Inelastic Static Isogeometric Analysis and 3D Design with Advanced Spline Techniques with Geomiso TNL: a New Hybrid Cloud-based CAD/CAE Software

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Key Words: *Isogeometric analysis, Finite element analysis, Computational structural mechanics, CAD, T-splines, NURBS, Patch, Material nonlinearity, Cloud-based software, Industry applications*

In this paper a recently developed cloud-based simulation platform (www.geomiso.cloud) is proposed to help engineers and industries make more effective use of 3D design and isogeometric analysis with advanced spline techniques. Geomiso TNL fully integrates the industrial design of any product with its computational real-time testing by facilitating the geometry modeling within analysis, thus it can solve demanding structural engineering problems subjected to static loading conditions otherwise very challenging. Users can easily test performance, predict behavior, optimize durability, and improve efficiency of their products. This is the first time ever such a cloud-based software has been developed.

This online solution provides inelastic static isogeometric analysis and 3D design of complex multipatch structures with NURBS and T-splines. Material nonlinearity in combination with the isogeometric method has attracted increasing attention. Modern T-splines can accurately represent any geometry with their local refinement properties and overcome limitations inherent to NURBS by ensuring higher-order continuity across patches, while in practical circumstances, it is often necessary to describe domains with multiple patches, especially them with parts in which different material or physical models are to be used. Geomiso TNL directly utilizes the CAD file in its solver to perform a structural analysis without any intermediate steps of geometry clean-up or further mesh generation by using the same shape functions, namely splines, for both describing the domain geometry and building the numerical approximation of the solution. Thus, it maintains the exact representation of the geometry at any stage of the design process and eliminates geometric errors. This hybrid software provides parameterized geometries in the design, while its modern graphical user interface offers an innovative way to preserve the exact geometry at all refinement levels. As it is demonstrated in this paper with several industry applications, the developed platform is seen to handle these situations remarkably well.

Geomiso TNL is considered to be a comprehensive answer to today's simulation challenges and a viable alternative to finite element software packages, as it removes the barriers between design and analysis and represents major improvements, such as higher accuracy, robustness, and stability level, combined with cost-efficiency and instant access from a web browser. This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship, and Innovation, under the call «RESEARCH–CREATE–INNOVATE» (project code: T1EDK-04288).

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Isogeometric analysis of monoclinic 3D concrete printing Timoshenko beam

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Key Words: *Isogeometric analysis, monoclinic, 3D concrete printing, Timoshenko beam*

3D printable concrete construction techniques have been well developed in the past decade. 3D printable concrete can be used to build free forms and shapes of structural components. In this paper, the isogeometric analysis (IGA) of 3D concrete printing monoclinic curved beam is made. Timoshenko curved beam theory in three dimensions is investigated. Definitions, properties, formula, and algorithms of Non-Uniform Rational B-Spline (NURBS) curves are reviewed. Corresponding finite element weak forms, discretization, and IGA formulations are derived and developed. Several numerical experiments are carried out and results are in a good agreement with experimental data in literature. It is indicated that the proposed isogeometric approach is feasible, accurate, and efficient to conduct an in-depth analysis of 3D concrete printing monoclinic Timoshenko beam.

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Isogeometric Analysis of Seismic Response of Multi-storey Buildings Resting on Raft Foundation with EPS Geofoam Seismic Buffer

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Key Words: *Isogeometric analysis, Finite element analysis, NURBS, Geofoam buffer, Expanded polystyrene, Seismic isolation, Building, Foundation, Load mitigation, Earthquake*

Seismic isolation is a technique that has been used worldwide to protect not only building structures and their non-structural components, but also their content from the damaging effects of a strong earthquake. The use of expanded polystyrene geofoam fills for foundation in areas with intense seismic activity, such as Greece, has seen growing use around the world in urban environments. This geosynthetic product, which is manufactured into large lightweight blocks, can be used as a fill material for seismic isolation of buildings against combined static and seismic activity. The mitigation of seismic-induced dynamic earth forces by placing geofoam buffer is a recent geotechnical innovation. This paper studies this novel seismic isolation technique implemented on a real-world project, where geofoam was placed at a depth below the raft foundation of multi-storey apartment buildings in Greece. The behaviour of this integrated soil isolation-building system and the influence of the buffer on the reduction of dynamic forces has been investigated. Numerical simulations of transient response were carried out using both the Geomiso software and FEA programs on models of these buildings resting on raft foundation in sand beds of different stiffnesses, with and without soil isolation mechanism. Parametric investigations were also carried out to study the effect of EPS density and thickness on the buildings' seismic response. The numerical results indicate that geofoam compressible inclusions significantly reduce the total applied pressure on the ground and drastically increases the bearing capacity of the buildings in static and seismic condition. With the increasing time, the compression of geofoam increases, while softer EPS blocks produce more compression which takes more vibration energy by their deformation. Better results were obtained with NURBS-based isogeometric analysis with Geomiso software (www.geomiso.com), as it achieves higher accuracy and efficiency as far as the calculation of load carrying capacity and stress fields inside the layered soil body are concerned. EPS geofoam seismic buffer is proved to be a new more efficient alternative soil isolation medium for buildings, as it substantially reduces the earthquake energy transmission to the structure and its dynamic response during earthquake ground shaking, thus it improves the building damage from severe to slight with lesser deformation. This is a novel technique for improving the building's earthquake resistance, which combines speed, cost saving and safety, and leads to more efficient seismic isolation. This research and specifically the first author has been supported by the Alexander S. Onassis Foundation (G ZG 017/ 2010-2011).

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Modeling and Analysis of Real World and Industry Applications with Geomiso ISA: A New Hybrid CAD/CAE Software for Static Isogeometric Analysis with Plate Elements and Advanced Spline Techniques

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Key Words: *Isogeometric analysis, Plate Theory, Kirchhoff-Love, Mindlin-Reissner, Splines, Patch, Slab, Industry applications, Software, Cloud*

In this paper, we propose Geomiso ISA (www.geomiso.com), a new software for applications on static isogeometric analysis with plate elements and advanced spline techniques. It is based on the isogeometric method, the powerful generalization of the traditional finite element method, which, in combination with the plate theory, has attracted increasing attention in construction industry over the last decade, as it achieves efficient design-through-analysis procedures and shows superior performance. Although NURBS are ubiquitous in CAD industry, the most promising spline technology is T-splines, which overcome limitations inherent to NURBS, ensure higher-order continuity across patches and permit local refinement.

The recently developed Geomiso ISA program is not just a plug-in, but a both on-premises and cloud-based software solution, applicable to real world and industry applications, which provides static isogeometric analysis with plate elements. It is used to simulate spline models of slabs and analyze their strength and behavior, while it has many features in common with both FEA software and design programs. This solution addresses the rising industrial need for seamless integration of computer-aided design and computer-aided analysis, while it appears to be more efficient to FEA software packages, as it facilitates the geometry modeling within analysis, eliminates geometric errors and achieves superior accuracy per degree-of-freedom with shortened computational cost. It offers an innovative way to merge geometric design with mesh generation into a single procedure by designing, with its modern user interface, slabs as tensor product grids in contrast to design programs.

Real world and industry applications on thin (Kirchhoff-Love) and thick (Mindlin-Reissner) plates are demonstrated with a comparison between Geomiso ISA and FEA programs, and between plate and hexahedral elements. We compare the accuracy of the numerical results, such as displacement, strain and stress fields, and the stiffness matrix assembly and solver time for analysis of typical slab types widely used in construction. We carry out parametric investigations on the effects of polynomial order, multiplicity and continuity of basis and shape functions, as well as on the number of control points and knot spans. This hybrid software represents improvements over finite element software packages, as higher accuracy, robustness, and stability level are accomplished.

This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship, and Innovation, under the call «RESEARCH–CREATE–INNOVATE» (project code: T2EDK-00703).

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Modeling and Analysis of Real World and Industry Applications with Geomiso SEA: a New Hybrid CAD/CAE Software for Inelastic Static Isogeometric Shell Analysis and 3D Design with Advanced Spline Techniques

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Key Words: *Isogeometric analysis, Shell Theory, Kirchhoff-Love, Mindlin-Reissner, Splines, Patch, Complex geometries, Industry applications, Software, Cloud*

In this paper the new Geomiso SEA software (www.geomiso.com) is proposed for applications on inelastic static isogeometric analysis with shell elements and advanced spline techniques. This hybrid program is applicable to real world and industry applications, while it satisfies the rising need for technical software of dual CAD/CAA nature. It is based on the isogeometric method, which has attracted a lot of attention for solving boundary value problems, as a result of using the same shape functions, means splines, for both describing the domain geometry and building the numerical approximation of the solution. T-spline-based isogeometric shell analysis has attracted increasing attention in automotive and aerospace industries, as it efficiently handles geometries with patches, discontinuities, and irregularities, while T-splines can design any geometry no matter how complex it is. Geomiso SEA is not just a plug-in, but a both on-premises and cloud-based software solution, which is used to simulate spline models of complex structures, or machine components, for analyzing their strength and behavior. This hybrid program, used for both design and analysis, has many features in common with both FEA software and design programs. It offers an innovative way to merge geometric design with mesh generation, by creating, with its modern graphical user interface, 3D models as tensor product grids. The utilization of the exact mesh for analysis eliminates geometric errors, while there is no need of repeating the geometry design for refinement purposes. In contrast, the standard finite element technique of remeshing with more and smaller elements, not only cannot fully utilize the available data of the exact mesh, but also makes engineers unable to benefit from advanced spline techniques, which are proved a mighty tool for IGA. Real world and industry applications on both thick (Mindlin-Reissner) and thin (Kirchhoff–Love) shells are demonstrated with a comparison between Geomiso SEA and FEA programs, and a comparison between shell and hexahedral elements. We compare the matrix assembly and solver time, as well as the accuracy of the numerical results. Parametric tests were also performed on the effects of the polynomial degree of the basis functions, and the number of patches, knot spans, control points, and integration points. This unique solution for seamless integration of the industrial design of shell geometries with its computational real-time testing, appears to be preferable to FEA programs, representing major improvements, such as higher accuracy, and considerably reduced computational time.
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Robustness Criteria Analysis for an Isogeometric-based Robust Shape Optimization Scheme of a Disc-pad System under Dynamical Criteria

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Key Words: Robustness, Multi-objective optimization, Iso-geometric formulation, Brake system

Robust shape optimization is a method to generate optimal geometries of mechanical parts with respect to performance objectives which depend on the application, while taking into account uncertainties linked to their manufacturing process or material properties. Such uncertainties can be understood as small perturbations of the design variables. Previous works have investigated approaches based on Efficient Global Optimization (EGO) with Expected Improvement (EI) criteria calculated using the worst case in terms of uncertainties [1], but these do not enable exploration of the entire Pareto front. Other studies have aimed to describe robustness as an additional theoretical optimization objective [2, 3].

Based on this approach, the presented work exposes an efficient way to thoroughly quantify robustness as an objective function. We apply such robustness criteria to a disc brake system under dynamical performance criteria, in order to determine a set of Pareto solutions which are the least sensitive to the design parameters' uncertainties.

The main optimization goal is minimization of squeal noise generated by the brake system which is expressed through Complex Eigenvalue Analysis (CEA) of the the dynamical model. A simplified model of the disc brake is advantageously constructed with the Isogeometric Analysis (IGA) formulation which is well-suited for optimization problems where numerous evaluations of the objective function are needed, leading to extensive use of numerical model calls.

A robustness criteria established on precise evaluation of the local variance of the output in the neighborhood of a solution is proposed and its effectiveness is discussed. In light of high computational cost, this robustness objective is coupled with a Kriging meta-model optimization scheme. The efficiency of IGA in the framework of robust multi-objective shape optimization under dynamical criteria is also inspected.

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A microscopic cyclic plastic model for carbide-free bainite rail steel

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Key Words: *Carbide-free bainite, Multiphase, Plasticity, Martensite transformation, Ratchetting deformation*

Carbide-free bainite (CFB) rail is a new generation rail for heavy-haul railways. Under the stress-controlled cyclic loading, the deformation mechanisms of CFB rail steel are mainly dominated by the bainite ferrite, martensite, and retained austenite. A microscopic cyclic plastic model that incorporates the plasticity of each phase and martensite transformation of retained austenite is proposed to describe the ratchetting deformation of CFB rail steel. Since the film-like retained austenite is located between laths (bainitic ferrite lath and martensitic lath), it is assumed that the strain of retained austenite and surrounding laths is the same. The Olson-Cohen model [1] is used to consider the strain-induced martensite transformation. The Mori-Tanaka mean-field theory is used to consider the interaction between bainitic ferrite laths and martensitic laths. The evolution equations of internal variables controlling the evolution of the hysteresis loop are dependent on the current dislocation density. The dislocation-based lath model [2] is introduced, and the strength difference between bainite ferrite laths and martensitic laths is considered. The comparison between the simulated and experimental results demonstrates that the proposed model can reasonably describe the ratchetting deformation of CFB rail steel.

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A unified constitutive model coupled with a continuum damage model for simulation of a broad set of elevated temperature responses

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Keywords: *Unified constitutive model, continuum damage model, Isotropic damage, creep-fatigue interaction, long-term creep, stress triaxiality*

A unified constitutive model[1,2] (UCM) coupled with continuum damage models (CDMs) is developed for simulation of a broad set of high-temperature responses, including fatigue, long-term creep, short-term stress relaxation, creep-fatigue, and thermomechanical fatigue. The model development was motivated primarily by the fact that available constitutive models were unable to predict all these responses using a single set of model parameters. Two CDMs, Kachanov[3] and the isotropic damage[4], are evaluated by coupling these with a Chaboche type UCM to achieve the objective. Based on the strengths and limitations of the continuum damage models studied in predicting the elevated temperature responses, a modified Isotropic damage model is proposed. The parameter determination of such a complex UCM-CDM manually is difficult, hence a hybrid and automated parameter determination tool implementing gradient and genetic algorithm approaches is developed. The modified UCM is experimentally validated against a large set of high-temperature alloy responses. The modified UCM in simulating creep responses of a notched specimen is also demonstrated. Finally, the proposed UCM is evaluated by analyzing a thick cylinder under thermal transient loading[5] to demonstrate the modified UCM's applicability for the design and evaluation of high-temperature components.

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Accurate Spring-back Prediction with Subloading Surface Model

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Key Words: *Digital Twin, Nonlinear FEM, Elastoplastic material modelling, Spring-back.*

Digital Twin technology that predicts deformation, material change and other behavior occurring production process is highly demanded since reduction of physical prototype with virtual prototype enables the cost reduction in addition to the shortening die design cycle. The key technology is the prediction accuracy of spring-back mode and amount. However this aspect of technology was not sufficient in case of high strength steel stamping cases in particular.

The conventional elastoplastic constitutive equation assuming perfect elasticity inside of the yield surface has been used for elastoplastic analysis by nonlinear finite element method. On the other hand, the subloading surface elastoplastic constitutive equation has the basic structure that the plastic strain rate is always induced even in a low stress state.

With the elasto-plastic traditional constitutive equation, it was difficult to precisely predict the spring back behavior after deep drawing metal forming process, in which material behavior during re-yielding in the reverse loading state is important. In particular, the amount of spring back of high tensile strength steels with initial yield stress of over 1 GPa, which are being used as automobile parts for weight reduction purpose in recent years, is bigger than conventional sheet metal and hard to predict.

Data calibration technology is also important for the accuracy. We developed the system that calibrates material constant and other parameters for the Digital Twin with CADLM system by learning data and internally generates ROM system for the simulation input parameter calibration in order to minimize the deviation between simulation result and nominal value of physically measured shape.

In this paper, we discuss on the implementation of subloading surface elasto-plasticity model into Marc implicit nonlinear finite element code and the effectiveness of sheet metal forming analysis using the subloading surface model in Marc which describes elasto-plastic material behavior even in reverse loading state accurately. This base Digital Twin model is subjected to optimization process for the accurate prediction performance enhancement.

An Efficient Parameter Estimation Method for Elastic-Plastic-Creep Simulation of Aluminum Alloys

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Key Words: *Elastic-Plastic-Creep Simulation, Aluminum Alloy, Constitutive Model, Parameter Estimation, Cyclic Loading, Strain Rate Effect, Temperature Effect, Thermo-Mechanical Fatigue*

Automotive engine components made of aluminum alloys are often subjected to loading in a high-temperature range that exceeds 1/2 of the melting temperature T_m of aluminum alloys. Therefore, the strength reliability of the aluminum alloy components should be evaluated by conducting elastic-plastic-creep finite element analysis (FEA). However, in fact, elastic-plastic FEAs have been conducted for the evaluation to avoid long-term product development time, because the elastic-plastic-creep FEA requires long-time creep tests under at least three stress levels at several temperatures to determine material constants. This is not a favorable situation to ensure the strength reliability of the aluminum alloy engine components. In this study, we propose an estimation method for the material constants used in a creep model for an aluminum alloy without conducting any creep test. The method utilizes stored heat cycle test data that are closely related to the strength reliability evaluation for aluminum-alloy engine components. The research and development departments of car companies often have stored a lot of test data related to practical use even though they do not have enough time to carry out creep tests. In addition, we introduce the "plasticity-creep separation method" [1], [2] which employs the estimated creep material constants to obtain time-independent stress-elastoplastic strain relations. Using these relations, the material constants for the plastic model considering the kinematic hardening can be estimated systematically. The elastic-plastic-creep simulations of time and temperature dependent cyclic deformations of the aluminum alloy are conducted using the estimated material constants. The simulations successfully predict both the time and temperature dependent deformations.

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Classification and overall-assessments of plasticity models

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Key Words: *Chaboche model, Classification, Mroz Model, Sublosading Surface Model, Plasticity model, Two-surface Model.*

Various plasticity models, i.e. the Choboche model[1], the multi-surface model[2], the two surface model[3] and the subloading surface model[4], etc. have been proposed hitherto. In this presentation, the mathematical-physical structures of these models are classified from the aspects of the yild surface, the existence of elastic domain, and their mechanical features are classified first. Then, the advantages and disadvantages of these models are analyzed comprehensively from the aspects of the description of monotonic-cyclic loading behavior, the mechanical ratchetting behavior, the stress amplitude, the unloading behavior, the efficiency of computation, etc. Consequently, the overall assessment of these models will be provided for the valuable information when the industrial engineers choose the suitable plasticity model for their mechancal design.

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Constitutive behaviour of viscoplastic materials under a wide range of strain rates and elevated temperatures

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Key Words: *Mechanical Behaviour, Constitutive Model, Strain Rate, Working Temperature.*

Thermal cycling reliability tests, as well as cyclic temperature changes caused by switching on and off and changes in ambient temperature during service, impose typical thermomechanical coupled physical fields on the solder joints, which significantly affects the mechanical reliability of the solder joint and the performance of the electronic device under the service conditions. To address the dwelling stages at low and high temperatures, an improved constitutive model is proposed in this study based on the unified creep and plasticity theory to describe the uniaxial mechanical behaviour of viscoplastic materials subjected to a wide range of strain rates and elevated temperatures. In the usual service condition of electronic devices, the strain rates of Sn3.0Ag0.5Cu (SAC305) solder material are far less than 1.0 s^{-1} at which the creep deformation is dominant, especially at higher working temperatures. However, the strain rate could range from 1.0 s^{-1} to 300 s^{-1} under drop impact in electronic packaging structures. The working temperature of solder materials is elevated above the room temperature up to 125°C as requried by the reliability standard for electronic packaing structrures. This is drawing more attention due to lack of experimental data, especially on dynamic mechanical properties of lead−free solder alloys. In extreme impact conditions, the solder material may experience even higher strain rates. As different mechanisms dominate the respective regime of strain rates, the developed constitutive model is calibrated to be applicable to most of the strain rate regimes by properly considering the coupled effect of creep and plasticity. Moreover, the parameters in the proposed model are defined with clear physical meanings and reasonably determined by regression to the published experimental studies. Lastly, the developed model is validated against experimental results at different elevated temperatures and also compared with other constitutive models, including the power-law equation for creep deformation at low strain rates and the Johnson-Cook model for plastic deformation at high strain rates. It is concluded that the proposed model is more generalized and capable of predicting uniaxial mechanical behaviour of SAC305 solder at low, medium and high strain rates from room temperature up to 125°C with reasonable accuracy.

Energy-Based Thermo-Mechanical Fatigue Life Prediction of Ferritic Stainless Steel for Exhaust Manifold

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Key Words: *Thermo-mechanical fatigue, ferritic stainless steel, energy-based life prediction model, plastic strain energy density*

In this work, thermo-mechanical life prediction of ferritic stainless is conducted using the energy-based method. As ferritic stainless steel is commonly used to high-temperature structures such as the exhaust manifold in automotive, it is apt to be exposed to thermal cycles[1]. Under that condition, thermo-mechanical fatigue can cause the failure of the structure induced by constrained boundary conditions. To evaluate the thermo-mechanical fatigue life appropriately, the accurate cyclic material property and life prediction model are required. Chaboche unified visco-plasticity model is established as the cyclic material property to incorporate the time-dependent behaviour in high-temperature[2, 3]. The isothermal tensile, low cycle fatigue tests are conducted to validate the determined cyclic material property. Thermo-mechanical life is evaluated using the energy-based life prediction model that the plastic strain energy density is used as the damage factor. It shows good agreements by comparing the predicted life and results of the thermo-mechanical tests using the V-shaped specimen.

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High-order strain gradient cyclic plastic model considering the interaction of microstructure evolution and size effect

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Key Words: *Sample size effect; Grain size effect; Strain gradient; Stress relaxation; Cyclic plasticity*

Size effects of both the sample and the grain on the cyclic torsion of micro-scale copper wires have attracted extensive attention. We constructed a high-order strain gradient cyclic plastic model to consider the coupling effect of microstructure and strain gradient. With a 3D element that separates the gradient field solution and the description of mechanical behavior, the simulation of cyclic torsional experiments of copper micro-wires was implemented into ABAQUS to reveal the change of strain gradient distribution with the cycle numbers in different working conditions. By introducing the intrinsic length of material and the average characteristic length of microstructure that evolves with the cumulative plastic strain, the anomalous Bauschinger effect, and the cyclic hardening characteristics[1-3] in symmetric cyclic torsional experiments were simulated. In addition, the internal stress conjugated to strain gradient was introduced into the back stress evolution, and the increase of mean stress relaxation with decreasing the sample size and grain size in the asymmetric cyclic torsional experiments[3] was simulated reasonably. This proposed model explains the influence of the material characteristic length evolution and strain gradient distribution on the cyclic torsion of micro-scale copper wires.

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Interlaminar Fatigue Strength Prediction of CFRP Based on Inelastic Two-Scale Analysis Method

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Key Words: *CFRP, Interlaminar, Delamination, Fatigue, Multiscale*

Carbon fiber-reinforced plastics (CFRPs) are used in various fields because of their high specific strength, high specific stiffness and high corrosion resistance compared to general metallic materials. Since CFRPs are composite materials in which unidirectionally reinforced resin sheets (laminae) are laminated multidirectionally, delamination can occur between laminae while they experience cyclic loads. Such delamination should be considered when designing CFRP structures because it can cause significant decrease of strength and stiffness of CFRPs.

In order to evaluate the delamination of CFRPs due to cyclic loads, it is important to know the interlaminar fatigue strength. For this, two kinds of testing methods have been conducted [1]. One is the four-point-bending fatigue test using L-shaped specimens, and the other is the flatwise tension fatigue test. However, the analysis method to predict interlaminar fatigue strength of CFRPs has not been established yet.

In this study, a prediction method for interlaminar fatigue strength of CFRPs is proposed based on an inelastic two-scale analysis method [2] combined with the Coffin-Manson law [3, 4]. First, the flatwise tension test of a CFRP is simulated using the two-scale analysis method, and the distributions of microscopic viscoplastic strain occurring at resin parts in micro-structures (unit cells) are examined. Then, the maximum value of microscopic viscoplastic strain is applied to the Coffin-Manson law for the resin to predict interlaminar fatigue life of the CFRP. It is shown that the proposed method is successful in predicting the interlaminar fatigue strength of the CFRP.

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Modeling of Cyclic Hardening with the Effect of Maximum Plastic Strain under Pre-loading and Ratcheting

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Key Words: *Cyclic Plasticity, Constitutive Model, Cyclic Hardening, Pre-loading, Ratcheting*

An extended evolution equation of cyclic hardening was proposed to include the effect of the maximum plastic strain induced by pre-loading and ratcheting. A set of evolution equations was also proposed for a plastic strain surface to properly evaluate the cyclic plastic strain range in the presence of pre-loading and ratcheting. The extensions were made by decomposing the plastic strain rate into the maximum and cyclic plastic strain rates.

The extensions were verified by performing uniaxial cyclic tests of 316 stainless steel at 600ºC, in which cyclic loading with a constant strain range was accompanied by either pre-loading or strain-controlled ratcheting. These experiments noticeably exhibited the effect of maximum plastic strain on the evolution of cyclic hardening.

The experiments were simulated using a constituive model with the extensions in addition to the resetting scheme proposed recently [1, 2]. Strain-range variable tests of 316 stainless steel at 600ºC [2] were also simulated. All the tests were accurately simulated. The extended equations were further used to discuss the effect of maximum plastic strain in light of experiments in previous studies.

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Subloading Surface Constitutive Model for Soils and Implementation into General Purpose CAE Code

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Key Words: *Soil, Subloading Surface Model, Cyclic plasticity, General Purpose CAE Code, User subroutine*

The history of plasticity started in the study of deformation behavior of soils by Coulomb when he proposed the yield (failure) condition of soils by applying the friction law proposed by himself. Thereafter, the leadership of soil plasticity was superseded by the metal plasticity. One of the reasons would be caused by the fact that soils exhibit various complex plastic deformation behavior. For example, the bulk modulus of soil increases upon pressing. Also, when the preconsolidation stress is exceeded, the stiffness reduces dramatically while the stiffness increases upon unloading. At failure, there is no resistance to shear, and stiff clays or dense sands are dilatant.

Over the years, many formulations have been used, including linear elastic, nonlinear elastic, Drucker-Prager or Mohr-Coulomb, and Cam-Clay and variations thereof. Take general purpose CAE code Marc (MSC Software [1]) as an example, the material models available for soil modeling are linear elasticity, nonlinear elasticity, the Cam-Clay model, von Mises, linear Mohr-Coulomb, parabolic Mohr-Coulomb, orthotropic elastic, and exponential cap model.

The incorporation of the subloading surface model is of crucial importance for the constitutive equation of soils because the remarkable softening behavior occurs in soils and thus the excessively high peak stress is described by the conventional plasticity model in soils. Explicit constitutive equations of soils will be described in this study, based on the elastoplastic constitutive equations.

In this study, a user subroutine of subloading surface soil model is implemented into Marc, and several fundamental problems are analysed to confirm its validity. Also, footing settlement problem is analysed to show the applicability of this model is verified by comparison with the test data for sand grounds with high friction property.

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Very Low Cycle Fatigue Crack Growth Simulation in a Pipe, Part I: Appropriate Cyclic Hardening Modeling

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Key Words: *Circumferential cracked pipe, very low cycle fatigue crack growth simulation, 3-D FE debonding technique, Chaboche combined hardening model*

The fracture behaviour for cracked pipes under seismic loading is an important part of the structural integrity for nuclear power plant. Seismic loading consists of the dynamic loading (strain rate effect) and large-amplitude cyclic loading (very low cycle fatigue loading). For the pipe material, the large-amplitude cyclic loading was more dominant effect on reduced fracture resistance than dynamic loading [1]. Many institutions performed the full-scale pipe under very low cycle fatigue loading [2]. The full-scale pipe test could accurately observe complicated pipe fracture behaviour, but had limitations of time and cost. The finite element (FE) damage analysis is numerical method that can simulate the crack growth under very low cycle fatigue loading using minimal experimental data [3]. As for the reliable predicted results, the cyclic hardening model should be appropriately applied by FE analysis [4]. In the previous studies [5], the cyclic hardening model, such as the Chaboche model, was mainly applied to the non-cracked structures, and the parameters were determined from hysteresis loop under low strain range. However, the crack exhibits the wide strain range depending on the distance and high strain near the crack tip. The cyclic hardening model parameters could not be determined from the specific and high strain range hysteresis loop. In this study, the simplified cyclic hardening modeling was proposed by considering the characteristic of cracked structure. The proposed hardenig modeling was developed to simulate the crack growth for cracked pipe under very low cycle fatigue loading. The FE debonding analysis was introduced to verify cyclic hardening model. The test materials were SA508 Gr.1a low alloy steel (non-cylic hardenig material) and TP 316 stainless steel (cyclic hardening material) at room temperature. The cyclic hardening model verified applicability to C(T) specimen and through-wall cracked pipe using FE debonding analysis.

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Very Low Cycle Fatigue Crack Growth Simulation in a Pipe, Part II: Validation using Experimental Data

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Key Words: *Circumferential cracked pipe, very low cycle fatigue crack growth simulation, multi-axial fracture strain energy density damage model, FE damage analysis*

In this study, ductile tearing of circumferential through-wall cracked pipes under very low cycle cyclic loading was simulated by using multiaxial fracture strain energy damage model [1], and simulation results were compared with the pipe fracture test under four-point load-controlled cyclic load condition [2]. Two parameters in the damage model, multiaxial fracture strain energy and critical damage value, are determined by analyzing standard tensile test and monotonic pipe test using FE analyses. The load amplitude and load ratio effect on the plastic strain energy under low cycle fatigue loading was incorporated by the multiaxial fracture strain energy density. The load amplitude effect (failure cycle) was included from the relationship between the plastic strain energy per cycle and the failure cycle [3]. The load ratio effect was included from the Coffin-mason fatigue curve considering the mean stress correction factor based on the Walker model [4]. The proposed damage model was applied by simulating the crack growth for through-wall cracked pipe under very low cycle fatigue loading with different load amplitudes and load ratios. The cyclic hardening model used the Chaboche combined hardening model verified by FE debonding analysis in Part I [5]. The predicted results compared with the experimental crack growth and fracture surface data and were in good agreements.

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A Study of LES Coupling with Thermal Radiation for Actual Urban District

- Investigation of Temperature Boundary Conditions and Inflow Turbulence including Weather Disturbance in Summer-

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Key Words: *Thermal Radiation, Urban District, Large Eddy Simulation, Inflow Turbulence, Weather Disturbance*

As an extreme weather event, recently heatwaves often occur in various regions in the world. Elucidation of real state and mechanism of the resulting heat stress becomes more important in order to keep comfort living space. In the temperature and flow fields, not only the steady characteristics but also unsteady change should be clarified because temperature and turbulent fields vary intermittently and locally. The formation of the outdoor thermal environment in urban districts is related to various factors such as solar radiation, long-wave radiation, airflow, and heat conduction. Therefore, in order to comprehensively simulate such outdoor thermal environment, it is necessary to consider the related physical phenomena such as air and heat transport, and radiation. For the method grasping the unsteady change of turbulent field in the actual urban districts, some researchers show the method using Large Eddy Simulation (LES). However, it isn't considered interaction between turbulent field and heat transfer from urban surface. Also, many researchers show the estimation of convective heat transfer coefficient (CHTC) as the analysis of heat transfer from cooled and heated urban surface, but the obtained characteristics are limited for very simple shape. On the other hand, turbulent and thermal fluctuations at the meteorological scale such as foehn wind and sea breeze also have a significant impact on the thermal environment in the urban canopy. Therefore, the generation of inflow turbulence that considered the velocity and temperature fluctuations in the actual meteorological field is an issue. In the previous study, Kawai and Tamura [1] proposed a method of adding high-frequency fluctuation of velocity in the driver region to the results of a mesoscale meteorological model.

This study shows complicated turbulent flows including fine structures around urban surface and heat transfer process in urban canopy by LES coupling with radiation model, and evaluates the thermal environment in urban districts. As the inflow boundary condition including a fluctuation of temperature for actual urban district in summer, we investigated the generation of inflow turbulence with weather disturbance and time-averaged temperature by mesoscale meteorological model.

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Analyses of Local Severe Wind Suction on a Square-section Cylinder by High-resolution Simulation and Conditional POD Method

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Key Words: Negative peak pressure, Trailing-edge vortex, Proper orthogonal decomposition, Square cylinder

In the wind-resistant design of cladding system in the façade of buildings, local peak pressures have received a great deal of attention from both safety and economic point of view. Many techniques for estimating the peak wind pressure have been proposed. However, it seems that no consensus is reached about which method should be used for determining peak pressure for the design purpose of cladding components. The main reason may be the lack of full understanding of the space-time characteristics of peak pressures [1]. This study used the high-performance computer to obtain the high-resolution flow and pressure fields around a square cylinder at Reynolds number of 22,000 [2]. The local severe suction immediately upstream of the trailing edges is particularly emphasized. The minimum trailing-edge pressure coefficients have a close correlation in a streamwise length of approximately $0.1D$ (D is the width of the cylinder). On the basis of high-resolution simulation, the occurrence of small trailing-edge vortex is observed, which has highly concentrated vorticity and is responsible for the trailing-edge peak pressures. The trailing-edge peak pressure occurs immediately before the shear layer moves far from the cylinder and recovers to the symmetric state. Standard proper orthogonal decomposition (POD) is applied to discover the inherent spatial modes with sharp peak pressures upstream of the trailing edges. Instead of the 1st mode (corresponding to vortex shedding), the higher-order modes contribute significantly to the trailing-edge peak pressures, whose mode coefficients have harmonics of vortex-shedding frequency. As a variant of POD proposed recently, conditional space-time POD is valid in studying the average evolution of wind peak pressures. It further provides the relative phase and frequency ratio between the trailing-edge peak pressure and vortex shedding.

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Large Eddy Simulation for Fluid Structure Interaction of $H/\sqrt{BD} = 5$ Rectangular High-Rise Building

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Key Words: *Large Eddy Simulation, Fluid Structure Interaction, High-Rise Building*

The application of Computational Fluid Dynamics on the evaluation of wind load on actual building is investigated in some research [1]. The wind load simulation results conducted by Tamura et al. show pretty good agreement with the corresponding wind tunnel test results. In the design of high-rise buildings especially with the height over 300m such as high-rise buildings being planned in Tokyo, not only wind load but also wind-induced vibration of building are quite important factors to be investigated. They should be evaluated simultaneously through a series of simulations, but the accuracy of evaluation of the wind-induced vibration amplitude using Computational Fluid Dynamics has not been investigated well yet. Therefore, the accuracy of evaluation of the wind-induced vibration amplitude using Computational Fluid Dynamics is investigated in this study.

The target model building is the rectangular building with the side ratio D/B=2 and the aspect ratio $H/\sqrt{BD} = 5$ where D and B is the long and short side length of the rectangular section respectively and H is the height of the building. The oscillation conditions such as modal shapes, natural frequencies and mass/mass inertia are set using the corresponding wind tunnel test conditions conducted by Marukawa et al. [2] The WALE subgrid scale model [3] is used to simulate fluctuating small scale turbulence, and the boundary layer turbulence generated in the simulation is acting on the building model.

The windward, transverse and rotational amplitudes of the wind-induced vibration of the building model under the free vibration condition are evaluated for several reduced wind speeds. The simulation results are compared with the corresponding experimental results [2]. The flutter for the transverse direction is simulated at the appropriate wind speed, and the amplitudes of the wind-induced vibration in the low wind speed range for three directions also show good agreement with the test results.

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Large-Scale Two-Phase Flow Simulation using Building-Cube Method for Urban Flooding

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Key Words: *Two-phase flow, Hierarchical Cartesian Mesh, finite volume method, flooding*

Recent climate change has exacerbated flood risk, especially in urban areas. In contrast to rural areas, floods in urban areas exhibit more diverse and complex flow processes because the water flows around or within buildings and pieces of urban furniture. In the conventional numerical studies for urban flooding, one or two-dimensional models based on the shallow-water equations have been generally adopted because a three-dimensional model requires enormous computational cost. However, 1D or 2D models cannot simulate complex three-dimensional flow and unsteady fluid force acting on structures in urban areas.

Considering the background mentioned above, we propose a gas-liquid two-phase flow simulation method by the finite volume method using the building-cube method (BCM) [1-3], which is suitable for large-scale parallel computing. In BCM, the computational domain is divided into cubic regions called cubes. Each cube is divided at equal intervals, the same number of cubes is assigned to each core, and the spatial loop processing is executed for each cube for load-balancing. The cell-centered finite volume method based on the BCM has been applied to single-phase flow simulations and fluid-structure interaction simulations in conventional studies. Still, it has never been applied to gas-liquid two-phase flow simulations.

To validate the present method, we demonstrate 3D dam-break simulation and water immersion simulation inside the building during flooding and discuss complex three-dimensional flow and unsteady fluid force acting on structures.

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LES Analysis of Ventilation Performance and Wind Gust Occurrence for Strategic Urban Transformation

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Key Words: *LES, Urban Transformation, Ventilation, Wind Resilience*

There is an urgent need for ventilation improvement in urban areas in order to mitigate the risk of illnesses due to unexpected contagious viruses or airborne pollutants and improve the thermal environment in terms of heat stress reduction on individuals and achievement of a carbon-neutral society. These needs and the transformation of people's lifestyles will most likely bring a gradual or metabolic transformation of urban areas. Thus, it is important to investigate the performance of potential modifying strategies for existing urban space configuration. In the course of the evaluation, the safety in extreme weather events such as increasing landfalls of violent tropical cyclones needs to be carefully assessed at the same time. In this study, we evaluated near-ground ventilation performance improvement in an actual densely built-up urban area of Shibuya district in Tokyo, Japan, in various assumed changes in urban space configuration using large eddy simulation (LES) at the grid resolution of about 90 cm.

Firstly, we examined the average nature of the ventilation improvement in the traditional urban redevelopment model, comparing the current urban configuration and the future configuration where many mid and low-rise buildings are replaced with fewer high-rise buildings. The average flow rate near the ground (at approximately 10 m height) increased by about 20% as a result of the space reservation and wind induction to the streets by the high-rise buildings aligned in the wind direction. However, the maximum instantaneous wind speed also increased in those spaces, and thus, appropriate measures needs to be taken against the wind force damage. Also, the buildings located close to each other in the orthogonal to the the flow direction caused infavorable consequence in the downstream region such as significantly lowered ventilation and more intensified wind gusts.

To seek potential future urban transformation strategies, we performed an investigation on the local flow change around a triangle-shaped urban block composed of mid and low-rise buildings in the city center considering two redevelopment scenarios: the block is replaced with (i) one high-rise slender triangular prism surrounded by an open space and (ii) one mid-high wide triangular prism with a courtyard. Inflow turbulence for this simulation was generated using the meteorological model/engineering LES hybrid approach proposd by Kawaguchi and Tamura et al. (2019) [1], replicating the actual meteorological structure of Typhoon Hagibis (2018). Both cases created more organized flow patterns inside the canopy region and seemed to have better ventilation performance than the present case where the buildings with inhomogenuous heights and shapes in the block generate random small eddies. Concerning the wind resilience design, highly unsteady gusts were generated mainly around the building associated with vortex shedding in Scenario (i), while mean wind speed and gust levels increased along the leeward street in Scinario (ii). We are planning to quantitatively analyze more variations of building shapes and layouts regarding their effect on urban ventilation.

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LES around a Realistic City Block Designed Based on a Future City Concept

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Key Words: *LES, Super High-rise Building, Peak Pressure, Typhoon*

As a concept of the city in the future, it is proposed to create a city where super high-rise buildings and low-rise buildings are combined based on an open space with abundant greenery. In this case, it is necessary to have a plan that fully considers not only comfort (heat environment, wellness) but also disaster prevention.

In particular, in the case of considering safety under strong winds, a large-scale numerical simulation of CFD [1] is required, since it is necessary to simulate a complicated flow field by reproducing detailed shapes including green areas, terrain, low-rise buildings and high-rise buildings.

In this study, we introduce the numerical simulation for the flow field of the realistic city block model planned according to the concept of the future city, in the case of an actual typhoon hits.

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LES on Wind Pressure Acting on High-rise Building under Strong Wind Events of Typhoon

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Key Words:*Large Eddy Simulation, Inflow Turbulence, Weather Disturbance, High-rise building*

Recently, extreme large typhoon attacks urban city and the damage of building structure occurs. For estimating damage of high rise building, the strucutural response and wind pressure on attachment of building are revealed by using wind tunnel experiment and CFD techniques. In most of cases, inflow conditions using turbulent boundary layer which develops on smooth or roughness surface are used. However, in the most of cases of strong wind events, disturbance derived from meteorological field with change of air density and temperature affects the characteristics on peak value and fluctuation of wind pressure on buildings. Now, it is possible to reproduce meteorological turbulent structure of Typhoon by meso-scale meteorological model. Large computation with spatial resolution less than 100 m makes it possible to show fine spatial structure with several hundred meters scale and velocity fluctuation with several ten seconds. In additon, techniques for generating inflow condition with high-frequency fluctuation which is impotant for estimating unsteady change of wind pressure are developed.

This study clarifies the effect of meteorological disturbance on wind pressure of high-rise building by comparing the computational cases which are different in 2 inflow conditions respectively. The one is inflow condition based on turbulent boudary layer and the other is inflow condition based on the meteorological field of Typhoon. For the inflow condition based on the meteorological field, turbulence of actual urban canopy is also included by CUBE (developed by RIKEN R-CCS) [1] computation for large urban area. Then, the generated inflow data are connected to the calculation domain of tetrahedral unstrucrture grid and wind pressure on actual high-rise buildng. Finally, the effects of large-scale flctuation derived from meteorological disturbance on wind pressure of high-rise building are revealed.

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Local Peak Pressure on Super High-rise Building in Actual Urban Area

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Key Words: *LES, Super High-rise Building, Peak Pressure, Conical Vortex*

In previous researches, the mechanism of the occurrence of local peak suction on single cylinder building model in turbulent flow has been investigated [1,2]. In this study, characteristics and cause of local peak pressure observed on the surface of a super high-rise building in an actual urban area are discussed through a relationship with the flow characteristics.

Large Eddy Simulation (LES) of high dense area in central Tokyo including several super high-rise buildings is carried out with the turbulent inflow boundary condition [3]. A distinctive wind pressure distribution with large negative pressure is observed at the windward corner on the sidewall of the target building. In the trace of pressure fluctuation at this point, very large suction peaks appear occasionally.

Based on computational results, the relationships between the flow characteristics and the pressure characteristics are analyzed. The wind speed at a point close to the windward corner increases before the peak suction occurs. It is found that strong flow separation generated from the windward building accelerates the conical vortex formed at the windward corner, which induces the peak suction.

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Study of Aerodynamic Characteristics of Eccentric Tapered Square Cylinder – Analysis of Flow field using BCM

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Key Words: *Aerodynamic, Tapered square cylinder, eccentricity, torsional vibration, BCM*

Due to improvement of construction technology in recent years, the number of construction cases of buildings with various plane shapes is increasing. Based on this tendency, in this study, we made a square cylinder model that has the plane whose upper part is eccentric and tapered in three stages as a trial. Generally, such structure is considered to advantageous for vortex-induced vibration, but there are concerns about the effect of torsional vibration due to the eccentricity of the upper part. In this research, we check the flow field and exam the effect of torsional vibration and vortex-induced vibration of this building using CUBE (Complex Unified Building Cube Method). CUBE is a simulation framework which has orthogonal grid system consisting of cubes and elements called cells that divide them, and each cube has a mesh system consisting of the same number of cells. CUBE can generate mesh automatically and calculate with high parallelization efficiency. For more information on CUBE, please refer to the following paper ([1]). This research is expected to expand the range of plane shapes that can be constructed in the future.

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Wind Pressure Characteristics of High-rise buildings in Middle and High-height Urban Areas Spread over Local Terrain

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Key Words: *Wind Pressure Characteristics, High-rise Building, Local Terrain, Inflow Turbulence*

The Akasaka area, which is adjacent to the green areas such as the Akasaka Imperial Property, the Hie Shrine, and the Sotobori area, is densely built with middle and high-rise buildings over the local terrain. It is important for wind resistance design to understand what kind of strong wind blows during a typhoon in such an urban area and the wind pressure acts on the buildings.

In this study, we focused on the wind of the wind direction SSE observed during Typhoon Lan (2017). We clarified the relationship between the wind flow field around buildings and the wall surface pressure by LES. The inflow turbulence obtained by the meteorological analysis and CFD for wide area was applied to the inflow boundary condition of LES.

Based on this result, we report the results of the effects of micro topography and trees on the wind flow and the wall surface pressure, and the characteristics of wind pressure acting on the uniquely shaped façade.

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WRF-LES Simulation of Wind Flow over Rough Urban Surface during Typhoon Lan (2017)

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Key Words: *WRF-LES, Typhoon, Urban Area, Mean Wind Speed, Wind Speed Fluctuation*

In an LES (Large-Eddy Simulation) to evaluate the wind load acting on buildings, the turbulent boundary layer flow is typically set as the inflow data. However, the effect of meteorological disturbances due to large-scale flow structures cannot be considered sufficiently in this method. Attempts have recently been made to generate LES inflow data that include the effect of meteorological disturbances by using meteorological models; further advancement of wind load evaluation using LES is expected. In a previous study, we indicated that the meteorological model overestimated the mean wind speed in an urban area because of an underestimation of ground surface friction (Nakajima et al., 2021). The prediction accuracy of meteorological models in urban areas needs to be improved to generate LES inflow data that include the effect of meteorological disturbances adequately.

In this study, we investigated the influence of the ground surface boundary conditions of the meteorological model on the accuracy in predicting the mean wind speed and wind speed fluctuation in an urban area. Two types of ground surface boundary conditions (Cases 1 and 2) were created. In Case 1, the roughness length for the urban area was set to 0.5 m uniformly (default setting), whereas in Case 2, the spatial distribution of roughness length for the urban area was set based on the urban geometry (Kanda et al., 2013). In Case 2, the roughness length in the central part of Tokyo was much larger than 0.5 m and ranged from approximately 4 to 20 m.

We performed wind flow simulations in the central part of Tokyo during Typhoon Lan (2017) using WRF-LES (LES mode of Weather Research and Forecasting model) with the created ground surface boundary conditions. The simulation results were compared with observation data at multiple locations. By setting the roughness length based on the urban geometry, the accuracy in predicting the mean wind speed in the urban area was improved significantly. However, in both cases, WRF-LES underestimated the turbulence intensity, especially near the ground surface.

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A Deep Convolutional Neural Network Approach as Surrogate Model for Topology Optimization

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Key Words: *Topology optimization, finite element method, deep learning, neural network, surrogate model*

It is widely recognized that traditional topology optimization (TO) method can be time consuming, mainly due to the finite element analysis (FEA) embedded in the iteration. In the past few years, the rise of deep learning (DL) has been driving the researchers to adopt artifical neural network (ANN) as a surrogate model to accelerate TO [1-3]. However, most research focus on treating the whole TO process as a black box, taking its inputs (boundary conditions, volume fraction, etc.) and outputs (the optimized structure) to train the surrogate model. This paper propose another angle to approach the problem, which is to focus mainly on the most time-consuming FEA part in the TO process. There are a number of surrogate models existing for structural FEA [4]. In this paper, an encoder-decoder convolutional neural network (CNN) is trained using data generated from the FEA module in the 88-line matlab code implementing the classic solid isotropic material with penalization (SIMP) method [5]. The trained network takes the boundary conditions and element densities as inputs and output the compliance of each element. Then, the compliance information is fed into the traditional TO numerical optimizer to derive the final optimized structure.

The main advantages of the proposed method are listed as follows.
1) The numerical optimizer is kept in the TO process. Therefore, the structural disconnection reported in other research [1,2] is naturally avoided.
2) By performing downsampling and upsampling in the CNN, the proposed method has a certain degree of generalization ability.
3) Future research may grow on the idea of seperating the two components of TO. For example, training another surrogate model for the numerical optimizer, and combining it with the FEA surrogate model to achieve further acceleration.

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Form-finding of Discrete Surfaces with Given Edge Lengths by using Force Equilibrium Method

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Key Words: *Discrete surface, Form-finding, Force equilibrium, Edge length*

This paper presents a practical algorithm for the form-finding problem of a discrete surface constructed by triangles with given edge lengths. This problem could have many applications, e.g., mathematical visualization, geometry processing, and architecture.

Theoretically, solutions for such form-finding problems always exist, and these solutions are not unique [1]. This characteristic enables the studies on surface deformation [2], for instance. This also gives us the chance to design a preferable shape in architecture, which is to find the shape as close as possible to the target shape designed by architects.

In many conventional methods of shape design, this geometry problem is transformed into a mechanical problem, where the edges are replaced by springs. The spring energy is then defined in terms of the difference in edge lengths, and the equilibrated shape is determined by energy minimization. However, the optimizer could get stuck in local minima, and results in an undesirable shape with local bumps and dips [3].

In this paper, we present a force equilibrium method for finding the final shape with given edge lengths. The edge lengths could be determined by using Ricci flow or other algorithms so that the surface has the specified geometric properties, such as uniform (discrete) Gaussian curvature [4]. The linear stiffness is used to predict the shape deformation in the iterative algorithm. Moreover, its pseudo-inverse is applied to compute the least-square solution for the system without boundary conditions.

Starting from the target shape, while driven by the unbalance forces due to differences in edge lengths, the proposed method enables the system to settle down quickly to the final shape having exactly the given edge lengths. More importantly, numerical examples demonstrate that the final shape is smooth and close to the initial design.

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Generating Topology-Optimized Shapes with GAN: Design support framework providing diverse shapes

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Key Words: *Topology optimization, GAN, Deep learning, CNNs, SIMP method, OC method*

We propose a new framework for more diverse design support by generating Topology-optimized shapes with GAN. In recent years, Topology-optimized shapes have been used to create attractive forms in the architectural field, as seen in the "Qatar National Convention Centre" designed by Arata Isozaki. Topology optimization has a high affinity with digital fabrication and is expected to be applied as architectural and structural design. In addition, many studies on structural design and form-finding for structural optimization by machine learning have been reported. However, a mainly progressive area of machine learning is image processing, and it is difficult to apply learning to extract features to other data structures.

Therefore, pixels in image processing and continuum elements in topology optimization can be considered as the same data structure, and thus topology optimization can be applied to deep learning using convolutional neural networks[1]. By applying GAN to learn topology-optimized shapes, it is possible to continuously generate variety of shapes with these features.

In this study, topology optimization using the SIMP method is adopted, the design domain is divided by finite elements, and the optimization process is solved using the optimality criterion method[2]. The topology optimization problem is assumed to be a compliance minimization problem. GAN is a machine learning technique that consists of two deep convolutional neural networks (CNNs), a generator and a discriminator, which are trained simultaneously while competing with each other. Here, we use Conditional GAN (CGAN), which can give directionality to the generated results by providing the class information of the dataset, labels[3].

We perform deep learning using GAN based on the data collected by the topology optimization and attempt to output the shape from the generator network after training. In this study, we execute several numerical experiments to learn topology-optimized shapes using GAN. The numerical experiments show that the GAN can reproduce the topology-optimized shape and generate various shapes by interpolating the features of the topology-optimized shape through feature learning. These results demonstrate the usefulness of GAN for generating diverse design.

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Hanging Membrane Forms Formalized by Differential Geometry: Shell Membrane Theory and Variational Principle

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Key Words: *Hanging Membrane Forms, Shell Membrane Theory, Variational Problem*

This paper presents hanging membrane forms based on formulation of differential geometry and discretized form-finding analysis. A reversed hanging membrane form in which pure compression stress state generates by acting the self-weight resist to the gravity naturally, economical construction has been implemented in consideration of construction materials. A. Gaudi was a famous architect who designed the Sagrada Familia, he applied the hanging model as an experiment to the structural form of the Sagrada Familia. H. Isler who was a structural engineer in Switzerland has constructed a lot of thin shell structures with reversed hanging membrane forms by an experimental approach in 1960's.
Recently, form-finding analysis have been developed and actively researched in architecture and computer graphics fields[1], an equilibrium form of unreinforced masonry structure can be computed using thrust network analysis[2]. An unreinforced masonry is a self-supporting structure in which only compression stress generates as with a reversed hanging membrane form. It has been confirmed that the Thrust Network Analysis (TNA) is a useful method by constructing the actual masonry structure. Airy stress function can define a horizontal stress distribution and can be applied to find equilibrium forms with in-plane stress[3]. These equilibrium forms can be described by the discretized polyhedral mesh in isotropic geometry[4].
These form-finding analysis can be formalized by various aspects such as equilibrium equations and geometric variational problems. However, consistent formulation is desirable between mechanics and mathematics, because the problem of nonlinear equations to find a structural form is important to consider the region of existence of solutions obtained form-finding analysis and certainty of the generating strass state.
In this paper, we present formulation of hanging membrane forms described by differential geometry and shell membrane theory[5]. We indicate that essential objects in hanging membrane forms are two-way nets expressed as isothermic coordinates, and show some numerical results of form-finding analysis.

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Material Cost Minimization Problem for Aluminum Alloy Beam using Beam String Structure

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Key Words: *Aluminum Alloy Beam, Beam String Structure, Cost Minimization Problem*

Industrial-use aluminum alloy materials are excellent in the lightweight and corrosion resistant, but inferior to the stiffness and material cost than steels. When the aluminum alloy is used to a girder bridge, the member cross-section must be larger than that of the steel because the same deflection limit must be applied regardless of the material types, and it results in higher material costs. Therefore, the aluminum alloy materials are often used not in the bridge girders but in the bridge components such as guardrails and lighting posts [1]. In this study, we try to apply the aluminum alloy materials to Beam String Structure (BSS) in order to improve the stiffness and reduce the material cost. In the BSS, the girder is supported by the cables through the struts to generate the negative bending moments, which can increase the stiffness of the entire girder [2]. In this paper, superiority of the BSS made of the aluminum alloy material is clarified through a combination of topology optimization and material cost minimization problem.

Fistly, configurations of the BBSs were determined by the topology optimization using grandstructure method. Then, six types of the BSSs were adopted in the material cost minimization problem, with three cable diameters and the number of struts of 1 and 2. For comparison to the BSSs, a simple supoprted steel and aluminum alloy beam were also considered. The material cost is adopted by the relative cost per unit mass multiplied by the mass of materials, referring to the literature [3]. The cross-section of the beam and strut and the height of the strut were used as design variables. The height of the beam, the width and height of the strut, the distance between the struts, the yield and buckling stress, and the deflection limit were used as constraint conditions.

The material cost of the simple supported aluminum alloy beams was approximately 42% higher than that of the simple supported steel beams. On the other hand, the material cost of the BSSs made of the aluminum alloy material was equal to or lower than that of the simple supported steel beams. Regardless of the number of struts, the material cost decreased as the cable diameter increased. Furthermore, the relationship between the span length and material cost was investigated. In contrast to the simple supported steel beam, which no longer satisfies the constraint when the span reaches a certain length, the BSS made of aluminum alloy material satisfies the constraint even when the span increased by 80% compared with that of simple supported steel beam. These results suggest that the development of lighter weight and longer span structures using aluminum alloy materials can be expected.

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Non-parametric Design of Free-form Shells with Specified Horizontal Reaction Forces

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Key Words: *Free-form shell, Shape design, Projected stress, Pucher's formulation, Membrane theory*

Analytical shapes such as spherical shells and cylindrical shells are widely used for shell roofs covering large space of architecture. However, it is preferable that the external loads are transmitted to the supports mainly through the in-plane (membrane) stresses to fully utilize the material of thin surface. For the vertical self-weight, such shape can be obtained by hanging a membrane or cable net and inverting it to generate a convex roof surface. This process can be computationally simulated using the optimization approaches of designing free-form shells. Geometrical approaches based on graphic statistics can also be utilized for designing convex shapes of compression-only shell roofs. Miki et al. [1] proposed a design method of a parametric surface under self-weight utilizing the framework of Airy's stress function.

For a graph surface of a thin shell modelled using the membrane theory, static equilibrium of the in-plane forces is described by the stress components projected to the horizontal plane using Pucher's formulation or Monge's description. Accordingly, the formulations based on Airy's stress function, which is generally used for the plates, can be used, and the existence of stress function is to be investigated for ensuring equilibrium of the curved surface. However, the distributions of stresses projected on the plane can be directly specified allowing discontinuity without checking existence of the stress function [2].

In this study, the method proposed in Ref. [2] is extended, and the description of graph surface is converted to a parametric form to design surfaces with curved boundaries. The x- and y-coordinates on the horizontal plane are expressed by Bernstein polynomials of two parameters normalized between 0 and 1. Detailed formulations are presented for solving discretized form of vertical equilibrium equation by finite difference approximation on the parametric plane.

In the numerical examples, various shapes are found by specifying the distributions of stresses projected on the horizontal plane. Accordingly, we can specify the horizontal reaction force (thrust) that is an important design parameter for the supporting structure. It is confirmed that smoothness of the surface shape is maintained even when the normal stress is discontinuous in the direction perpendicular to its direction. A static finite element analysis is carried out to show that the stresses are sufficiently close to the specified values even considering the deformation under self-weight, if the restriction along the boundary is appropriately compensated by a forced in-plane deformation before applying the vertical loads.

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Optimization Problems with A Density-based Clustering Algorithm

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Key Words: *DBSCAN, Clustering, Descent method, Optimization problem, Solution space*

This paper presents optimization problems with a density-based clustering algorithm by obtaining all extremal values of solution space. In the architecture, designing building have to take account of several field such as architectural design, environmental engineering and structural engineering. In addition, as setting numerically priorities among design, usability and safety has difficultly, providing various solutions that are well evaluated is important. Thus, proposing not only a global optimal solution but also local optimal solutions in the optimization problem is important in optimization problems of building structure with multiple extremal values. The previous study has proposed the method that obtains multiple extremal values as optimal solutions utilizing a clustering method. This optimization enables us to obtain global and local optimal solutions efficiently by introducing a clustering operation to FA[1]. However, *k*-means method of partitioning clustering algorithms requires the number of clusters as a parameter of optimization problems. If the number of predetermined clusters is less than or greater than the number of extremal values in the solution space, finding some of the extremal values is missed. This is "the lucked of diversity of solutions". In this paper, we present the method combining hill climbing method for a local search method and DBSCAN[2] for a density-based clustering algorithm, which enables us to find all extremal values of the solution space for optimization problems without predetermining the number of clusters. The method consists of a few coordinating processes. Using Latin hypercube sampling, we initiate the process by generating the random data on solution space. Hill climbing method enables us to collect the generated data around external values, which is classified into clusters with DBSCAN in the following process. The results of our numerical experiments show that proposed method could identify extremal values for several benchmark functions[3] and a structural optimization problem[4] as the number of clusters. From these results, this method would allow us to grasp extremal values in the solution space, which structural optimization problems have high-dimensional variables, as the number of clusters. Moreover, this method would be able to present various solutions for structural and architectural design.

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The Reason Solving a Tension-compression Mixed Shell Form-finding is so Difficult and How to Solve it

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Key Words: *Airy's stress function, shell, form-finding, nonlinear least-squares method,*

In architectural design and structural engineering, membrane-shells that stand against the gravity by in-plane membrane stresses only have been paid a consistent attention. However, the built or computed membrane shells are typically in compression-only although there is no fundamental theory contrary to a mix of tension and compression. It is expected that overhanging anticlastic surfaces can be achieved with no bending action if the forms of tension-compression mixed membrane shells can be computed numerically.
The natures of the equilibrium equations of the pure-compression and tension-compression mixed types are surprisingly different because the former is elliptic while the latter is hyperbolic. The fact that the equilibrium equation becomes hyperbolic is making the tension-compression mixed form-finding a challenge.
This paper explains why solving the tension-compression mixed form-finding problem of membrane shells is so difficult and presents a powerful strategy to solve the problem numerically. In short, there is a high possibility there being no solution. Hence, a test method to determine/evaluate if the problem solved had a solution is needed. With the concept of the Airy's stress function to compute the forms of shells, when the problem has a solution, the Airy's stress function can be recovered with no loss of information from the computed shell. If the information is lost during the recovery, the problem is judged to have no solution. This concept can be beautifully realized with the nonlinear least squares method and the problem can be solved by the variable projection method briefly overviewed by Elden and Ahmadi-Asl, 2019[1]

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The Use of Three Solvers: IPOPT, SNOPT and MMA to Optimize the Shape of the Coating

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Key Words: *Shape Optimization, Spherical dome and Right helicoid, Gradient solvers, Optimal solution*

Each optimization program has special modules for calculation, which are based on several algorithms. Thus, the presence of a choice among the solvers contributes to the selection of the most suitable solution for any problem.

In this work two shells: spherical dome and right helicoid are calculated in the program Comsol Multiphysics in the module Shape optimization using three gradient methods: MMA (the method of Moving Asymptotes), IPOPT (Interior Point OPTimizer), which is based on the use of sequential quadratic programming (SQP) method and SNOPT (Sparse Nonlinear OPTimizer), which is based on the interior-point algorithm with a filter line search method.

The purpose of the study is to compare the three methods in detail with each other and choose the most optimal form for shape optimization. For each method, an analysis is carried out according to the following criteria: the speed of obtaining results and the greatest change in the shape geometry.

The main stages of the study are based on the following points: a study of the main functionality of solvers; modeling and further calculation of the shells with the assignment of special criteria in the programs under study; the overview of the obtained results and selection of the most optimal solver for calculation.

The solvers IPOPT and SNOPT are similar in structure, so the values obtained using these methods do not differ much, although the IPOPT method has managed to achieve the most optimal solution for shells. The smallest changes in geometry were observed using the method MMA.

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Topology Optimization of Structural Frames Considering Various Non-Mecanical Performance Formulated as MISOCP

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Key Words: *Topology optimization, MISOCP, Global optimal solution, Interior point method, Branch-and -cut method*

It is known that the topology optimization (TopOpt) problem of frame structures can be formulated as a mixed-integer second-order cone programming problem (MISOCP), when the compliance is minimized and the cross-section of each member is selected from a set of predetermined candidates[1]. An MISOCP problem can be solved globally with a branch-and-cut method (B&C) while global optimalty is mathematically guaranteed. When the B&C makes MISOCP a continuous problem, the resulting problem is a second-order cone programming (SOCP) problem, which can be solved efficiently with a primal-dual interior-point method. Previous studies have demonstrated the effectiveness of TopOpt by MISOCP for the simple stiffness maximization problem of medium-sized structural frames[2]. However, if we consider design and construction of real-world building structures, it is insufficient to optimize only the mechanical performance. In the latest research of such optimization approach, it is confirmed that various non-mechanical constraints, such as upper bounds for the member lengths, the number of nodes, lower bounds for the joint angle of members, can be additionally taken into account[3]. On the other hand, the density of members to each joint also affects the non-mechanical performance (especially constructability), but this has not been considered in previous studies.

In this paper, TopOpt by MISOCP with new constraints that take into account the density of the members by constraining the number of members connected to each node is considered. Furthermore, TopOpt is performed for various analytical models while not only proposed constraints but also various non-mechanical constraints considered in previous studies are simultaneously taken into account.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Augmenting Scientific Data using GANs

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Key Words: data augmentation, generative adversarial networks

The study of many scientific and engineering problems requires constructing predictive models of multi-scale and multiphysics systems. The recent explosion of scientific machine learning research has shown tremendous potential of enhancing new discovery in these complex systems. Yet the promise of most machine learning techniques relies on the availability of a large volume of high-quality training datasets, which are obtained through expensive experiments or simulations. Therefore, data augmentation techniques can be of great help for scientific machine learning problems. However, directly implementing data augmentation techniques originating from computer vision, can yield physically unacceptable data samples. We develop a new data augmentation technique based on generative adversarial networks (GANs). It can leverage different physics knowledge, e.g., governing equations, observable perception, and physics phenomena to improve the quality of the augmented synthetic data. We will demonstrate its efficacy by generating configuration samples of porous media with given constraints, and by augmenting spatio-temporal data using limited high-quality simulation results.

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Development, Learning and Optimization of Viscoelastic Laminated Composite Beams

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Key Words: *Composite beams, Viscoelastic materials, numerical simulations*

Composite beams have found increasingly more engineering applications due to their high specific stiffness and strength. Nevertheless, these problems present challenging modelling, mathematical, and numerical issues including heterogeneous and distinct anisotropic properties, high frequencies with potential resonance issues.

We present a mathematical model for describing dynamic vibrations of viscoelastic composite beams with laminated structures. We will mathematically analyse the model, investigate performance of the model, and learning and optimization of the model.

Learning Nonlocal Operators for heterogeneous material modeling

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Constitutive modeling based on the continuum mechanics theory has been a classical approach for modeling the mechanical responses of materials. However, when constitutive laws are unknown or when defects and/or high degrees of heterogeneity present, these classical models may become inaccurate. In this work, we propose to use data-driven modeling which directly utilizes high-fidelity simulation and/or experimental data on displacement fields, to predict a materials response without the necessity of using conventional constitutive models. Specifically, the material response is modeled by learning maps between loading conditions and its resultant displacement fields, so that the network is a surrogate for a solution operator. To model the material heterogeneity, integral neural operator learning methods are employed, which are resolution-independent and naturally embeds the material micromechanical properties and defects in the integrand. We demonstrate the performance of our method for a number of examples, including hyperelastic, anisotropic and brittle materials. As an application, we employ the proposed approach to learn material models directly from digital image correlation (DIC) tracking measurements, and show that the learnt solution operators substantially outperform conventional constitutive models in predicting complex material responses.

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Leveraging Machine Learning for Subsurface Modeling with Fractional-Order PDEs

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Key Words: Deep Learning, Fractional, Nonlocal, Subsurface, Anomalous

Data from both numerical simulations as well as physical experiments of subsurface flows reveal that contaminant tracer is often anomalous, with breakthrough curves and mean-square displacements exhibiting heavy, non-Gaussian tails characteristic of Lévy processes, the statistical properties of which are described by fractional-order models. We leverage recent machine learning approaches for inverse problems to demonstrate and compare the efficacy of fractional-order models and local models in a variety of datasets. Our results are both a novel application of machine learning approaches to model discovery for such applications and shed light on what type of models can be expected to accuractely describe subsurface flows in different materials.

Meta-Learning for Heterogeneous Materials: A Provable Nonlocal Operator Regression Approach

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Key Words: Neural Operator Learning, Representation Learning, Partial Differential Equation Learning, Meta-materials.

In this talk, we propose a meta-learnt approach for learning mappings between function spaces (operators), Meta-NOR, based on the nonlocal operator regression [1], to efficiently provide accurate model surrogates for in new and unknown governing law tasks. The proposed provably sample-efficient meta-learning algorithm uses a multi-task nonlocal operator regression model in the kernel space, which consists of two phases: (1) learning a common nonlocal kernel representation from existing tasks; and (2) transferring the learned knowledge to rapidly learn surrogate models for new tasks with different governing laws (such as with different constitutive laws or material parameters), where the governing laws could be possibly unknown and only a few test samples are provided. Under the linear kernel regression setting, a provable optimization-based approach is provided, with theoretically guaranteed transfer-learning error bounds. We apply the proposed technique in the context of meta-materials, showing that the meta-learnt kernel representation would greatly improve the sampling efficiency in new and unseen microstructures, compared to existing baselines. To handle more complex material responses, we further extend the proposed meta-learnt approach to the integral neural operator architecture [2,3], and demonstrate its performance on learning hidden governing laws of Darcy's flow.

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Nonparametric learning of kernels in nonlocal operators

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Key Words: Nonlocal kernel, Identifiability, Inverse Problem, RKHS

Nonlocal integral operators arise in various areas such as nonlocal partial differential equations, fractional diffusions, and nonlocal networks. An important topic is to learn from data the nonlocal integral kernel, which is often radial to achieve homogeneity. We introduce a nonparametric approach to yielding a convergent estimator of the kernel as the data size increases. A key ingredient is a new spare-aware regularization method to prevent over-fitting and overcome the inverse problem's ill-posedness. The method's foundation is the function space of identifiability, a system-intrinsic data-adaptive RKHS (reproducing kernel Hilbert space). Furthermore, the identifiability theory suggests that the inverse problem is ill-posed. Thus, regularization is necessary. We systematically study the spare-aware regularization with synthetic data, showing the convergence of estimators. We also apply our method to experimental data in peridynamics, for which we learn a homogenized nonlocal model.

Bayesian Model updating of Linear dynamic systems using complex modal data

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Key Words: *Bayesian Model Updating, Dynamic Condensation, TMCMC, Complex modal data.*

In the lifetime of structures, they may be exposed to damage that deviates their parameters to a new uncertain state. To predict these parameters, they must be updated using experimental data through various model updating methods. Among model updating methods, the Bayesian approach enables the exploration of all the probable models. Many approaches are available, like those that require the solution of the eigenvalue problem [1] and those that do not require the resolution of the eigenvalue problem [2, 3]. Most existing studies have assumed proportional damping, which gives real modal data, which is not the case always [4]. In this paper, a new Bayesian model updating methodology is proposed based on introducing system mode shapes, damping ratios and natural frequencies as additional uncertain parameters. A dynamic condensation technique is used to restrain the model updating problem to work on the observed degrees of freedom (DOF) field only. To decrease the number of uncertain parameters, system mode shapes are integrated out, and Transitional Monte Carlo Markov Chain (TMCMC) is used to sample from the posterior probability density function. The proposed approach has been applied to the 3-storey shear building model. Results show that the proposed methodology can predict the updated structural parameters in many cases, like the cases where the number of observed modes is greater than the number of observed DOF and if the observed modes are not the lowest-frequency modes.

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High Dimensional Bayesian Updating of Structural Dynamic Models with Reliability Methods

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Key Words: Bayesian model updating, Reliability analysis, Simulation techniques, Structural dynamics

Model updating of structural dynamical models using measured responses has an important number of applications in several areas. For a proper assessment of updated models all uncertainties involved in the problem need to be considered. In this regard, an approach for Bayesian model updating of structural dynamical systems involving multiple uncertain parameters and measured responses is presented. The proposed scheme relies on the use of structural reliability methods, where samples following the posterior distribution are obtained as failure samples corresponding to a specially devised reliability problem [1]. Subset simulation, a well known and widely applied advanced stochastic simulation technique, is adopted to generate the required failure samples [2]. The approach requires only minimal modifications of the standard formulation of subset simulation and it uses an adaptive strategy to select the threshold value that determines the last subset level. For an efficient numerical implementation, an effective parametric reduced-order model formulation based on substructure coupling for dynamic analysis is considered [3]. Due to the basis of the formulation, the approach does not make use of any problem-specific information and, therefore, any type of structural model can be considered. The performance of the proposed method is assessed numerically with an example problem involving a nonlinear three-dimensional bridge structural model with many uncertain parameters. The results suggest that the proposed approach is an effective tool to address Bayesian model updating problems involving complex structural dynamical models, measured response data and high-dimensional parameter spaces.

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Minimizing the Probability of Failure of Stochastic Linear Dynamical Systems via a Decoupled Approach

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Key Words: *Stochastic linear system, Reliability-based optimization, Decoupling*

Reliability-based optimization (RBO) offers the means for determining optimal structural designs while explicitly taking into account the effects of uncertainty on structural performance. While the advantages of RBO over deterministic design procedures are evident, its practical implementation is usually quite challenging from a numerical viewpoint. This is a consequence of the necessity of solving simultaneously a reliability problem nested in an optimization procedure, that is, a double–loop problem.

In view of this challenge, this contribution develops a most efficient approach for RBO for a specific class of problems. The focus is on the minimization of the failure probability of linear structural systems subject to Gaussian stochastic loading under a given budget constraint. The reliability measure considered here is the first excursion probability of the structure, which is a typical means for quantifying safety in stochastic dynamics. The proposed approach is formulated within the framework of the operator norm theorem, which allows full decoupling between optimization and reliability analyses [1]. That is, the classical double–loop approach for RBO is effectively broken and reduced to the solution of a single deterministic optimization problem followed by a single reliability analysis. Such an approach allows diminishing numerical costs by orders of magnitude when compared to a traditional, double–loop implementation. The application and capabilities of the proposed approach are illustrated by means of an example.

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Probabilistic Response Analysis of Nonlinear MDOF Dynamic Systems under Combined Multiplicative and Additive Excitations

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Abstract: The probabilistic response analysis of structures subjected to combined multiplicative and additive excitations is a challenging issue. The direct probability integral method (DPIM), as a novel method, has demonstrated its high accuracy and efficiency in the random variation analysis of nonlinear multiple-degree-of-freedom (MDOF) systems under additive excitation [1, 2], i.e., Gaussian white noise excitation. In this paper, the DPIM is extended to address the probabilistic response analysis of nonlinear MDOF dynamic systems under combined multiplicative and additive excitations. The first aim of the paper is to investigate the random vibrations of the MDOF dynamic system, showing the evolutionary process of probability density functions of the response and stochastic bifurcation. To further display the global dynamics of MDOF system, the second aim of this work is to obtain the attractors, and basins of attraction. By incorporating the generalized committor functions, the basins of attraction of system are generalized via DPIM and the dynamic integrity measures are then evaluated. In the numerical examples, the effectiveness of the proposed method is verified by comparing the results of Monte Carlo simulation.

Key Words: *Nonlinear MDOF dynamic systems, Multiplicative and additive excitation, Direct probability integral method, Stochastic bifurcation*, *Global dynamics.*

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Robust Design Optimization Under Uncertain Structural Parameters by Stochastic Simulation-Based Approach

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Key Words: *Robust design optimization, optimization under uncertainty, parameter uncertainty, genetic algorithm, mean–variance.*

The inherent uncertainty in the structural parameters directly affects the structural performance, and its variation may lead to improper designs and catastrophic consequences. When subjected to uncertainty, the structure design must be optimized to get an insensitive design using a Robust Design Optimization (RDO) technique. Such design aims to find a system design in which the structural performance is less sensitive (insensitive) to the uncertainty of the inherent structural parameter without eliminating them [1]. This is usually achieved by simultaneously minimizing the mean and variance of the structural performance function. Various RDO approaches, such as those based on Taylor series expansion [2] simulation-based methods [3], dimension reduction [4], and metamodel [1], can effectively take into account these uncertainties. However, the computational efficiency and accuracy in evaluating the mean and variance of the performance function remain a challenging task. To obliviate this limitation, a novel stochastic simulation-based approach is proposed in the present work. The proposed approach is built on an 'Augmented optimization problem,' in which design variables are artificially considered as an uncertain parameter. An unconstraint Genetic algorithm (GA)-based optimization approach is formulated to determine the optimal solution. As the mean and variance frequently conflict with each other, so to obtain the Pareto optimum, a linear scalarized objective function is adopted. To demonstrate the proposed approach, RDO of a four-bar and 10-bar truss structure is performed. The results obtained are compared with the conventional Monte Carlo simulation approach and confirm that the proposed approach yields accurate results. This paper allows the designers to design the insensitive structure systems by minimizing the variance of performance function. Moreover, the proposed RDO approach is not limited to the civil structures only, but it can also be enforced in the design of any realistic linear/nonlinear structures and systems such as machine components (like clutches, gears, etc.), aerospace, etc., having uncertainties in their geometry or material, such as the residual strain, modulus, thickness, density, etc.

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A Topology Optimization Method using Differential Evolution based on RBF Networks

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Key Words: *Topology optimization, Radial basis function network, Differential evolution*

Abstract The application of structural optimization is an effective method to create and design high-performance structures without relying on the designer's intuition, experience, or trial and error. In particular, topology optimization is used as the structural optimization method with the highest degree of design freedom. However, as the target problem becomes more complex, sensitivity analysis, which is essential for topology optimization, becomes more difficult.

In this paper, we propose valid methodologies to address that shortcoming. The density of the structure is expressed by placing equally spaced Gaussian functions in the design domain and superimposing them based on the RBF network. Furthermore, by using the height of the Gaussian function as a variable in the differential evolution calculation, the optimal structure is obtained without sensitivity analysis. Here, MLSHADE-SPA[1], which is competitive in solving large-scale global optimization problems, is employed as the differential evolution algorithm. With this method, we obtained the same optimal structure in the stiffness maximization problem as when using the conventional topology optimization method[2]. However, since the current program requires a huge computational cost, it is necessary to reduce the computational time. In future work, we hope to extend our method to some more complicated multi-physics problems such as thermal-fluid problem, electromagnetism problem, etc.

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Application of Genetic Algorithm for Parameter Design of Generative Adversarial Networks

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Key Words: *Generative Adversarial Networks (GANs), Genetic Algorithm (GA), Hyper-parameter*

ABSTRACT

Generative Adversarial Networks (GANs) are a kind of neural network frameworks presented by Ian Goodfellow et. Al. [1]. GANs has two neural network structure; Discriminator network and Generator network. Generator network generates prediction results and Discriminator network evaluates that the image is “real” or “fake”. GANs have been proved useful for semi-supervised learning.

In this study, GAN is applied for future image generation problem of walking pedestrians. The aim of this problem is to generate the continuous future images from their past images of walking pedestrians. The convolutional networks are adopted for both Generator and Discriminator networks in this study, instead of the fully connected network used in the previous study. Some experimental results show that the proposed algorithm is useful for future image generation of walking pedestrians.

For effectively applying the GANs-based algorithm for generating the continuous future images from their past images of walking pedestrians, however, there is one problem to be solved. The performance of the proposed algorithm depends on the hyper parameters and the number of images. For solving this problem, Genetic Algorithm is used in this study. The hyper-parameters of the Discriminator are fixed and then, the hyper-parameters and number of images for the Generator network are determined by Genetic Algorithm. The fitness function is defined by loss function of Generator network. Individual chromosome is composed of hyper-parameters of the network; number of hidden layers and activation functions at hidden layers, and numbers of input images and output images.

When the proposed algorithm is applied for future image generation of walking pedestrians, the hyper-parameters and the number of images for Generator network can be optimized automatically. Although number of hidden layers is 4 at both the original and optimized networks, the activation functions are changed. Besides, numbers of input and output images are also different at both networks. As a result, Perk Signal to Noise Ratio (PSNR) of the generated images is improved from 29.1 in the original network to 29.6 in the optimized one. Therefore, it can be concluded that the proposed algorithm can improve the hyper-parameters and number of images for the Generator network automatically.

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Application of Grammatical Evolution for Design of Control Program of Robot

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Key Words: *Grammatical Evolution, Backus-Naur Form (BNF), Control Program, Mindstrom.*

Robots has become widespread in various applications. For the effective use of robots, it is necessary to design a control program that is effective for the desired movement. Since it is difficult to define the control program of a robot manually, use of evolutionary computation (EC) for designing control program is studied widely. Grammatical Evolution (GE) [1], which is one of evolutionary computations, is designed for determining the function, program or segment of program satisfying the design objective. Although aim of GE is similar to Genetic Programming (GP) [2], GE uses simpler genetic operators than GP. In this study, GE is applied for design of the control parameter of travelling robot. GE defines the candidate solutions by set of binary numbers and update them by applying the genetic operators such as selection, crossover and mutation, which are similar to them in Genetic algorithm (GA) [3]. Translation from the set of binary numbers to function or program is performed according to the translation rules defined in Backus-Naur form (BNF).

A travelling robot moves along an oval course which is drawn on the paper. GE generates the control program of LEGO Mindstorm EV3. The part of the control program which is generated by Grammatical Evolution. The function SensorValue(S3)>90 means that the robot is on the oval course. In that case, the robot goes straight. If not so, the robot turns right. The simulation and the experimental results of the robot trajectory achieved small differences. The experimental result agrees well with the simulation one.

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Concurrent Multiscale Topology Optimization for Designing Displacement Inverter

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Key Words: *Topology optimization, concurrent multiscale optimization, displacement invertor, periodic microstructure. compliant mechanism.*

Structural light-weighting is vital for increasing energy efficiency and reducing CO_2 emissions. One of the mechanical structures that are used in numerous applications and can utilize lightweight is the displacement invertor. Displacement inverter is producing mechanical reaction as the reverse of the input actuating action. In this research, multiscale topology optimization of compliance mechanism is used to design lightweight displacement invertor. This is because compliant mechanisms, and in contrast to typical mechanisms that are coupled by rigid bodies, are flexible single-piece systems that achieve the desired movement through elastic deformation. Furthermore, reduced friction, wear, noise, and the ability to provide novel actuation, as well as ease of fabrication and assembly, are among the advantages of the use of compliant mechanism design concepts. Under the constraint conditions of the total area of the microstructures distributed in the macrostructure, the elastic response of the macrostructure, and the homogenization set of the periodic unit cells are used associated with the rigidity control rational problem (the ratio of the output and input displacements) of the design domain which is used as the objective function for topology optimization method. Topology optimization for material distribution is a crucial stage in the design of compliant systems. It aids designers in extending and fine-tuning a design with the optimal material distribution. It entails determining the shape and placement of a structure's cellular units, as well as the domain's connectivity. Binarization and intermediate pseudo density were investigated for the concurrent multiscale optimization of the rigidity control structures using solid isotropic material with penalization (SIMP) and evolutionary structural optimization (ESO). As a result, the effective properties obtained using the homogenization for the microstructure are evaluated with a dedicated finite element model, while the macrostructure's effective properties are calculated using a different finite element model. The adjoint approach is used to implement the sensitivity analysis efficiently for the concurrent design function in this study, which reduces the computational cost. The numerical examples showed a good design response of the microscale design with the spatial configuration and the boundary condition of the design domain on both macro and microstructure. Furthermore, this study found that addressing microscale design with the concurrent optimization process, it is possible to get a desirable spatial configuration of materials while reducing weight. the spatial arrangements for the various scenarios revealed an elaboration for distributing strain energy in the most efficient manner possible in relation to macrostructure design. As a result, the proposed design process has the potential to produce durable and new lightweight and porous displacement inverters' designs with unique and high adaptability of elastic property.

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Denoise in Reconstructed Point Cloud of Branch-Shaped Complex Structures using Clustering

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Key Words: *3D reconstruction, Clustering, DBSCAN, SfM, Point cloud, Branch-shaped complex structures*

Structure from Motion, which can reconstruct 3D point cloud, camera positions, and orientations using images of an object from different angles of view, has been widely used for visualization of structures and inspection of machined parts[1]. In this method, information other than that of the object in the image is also reconstructed. In order to remove noise, methods based on k nearest neighbors searching for reconstructed point clouds with simple shapes[2], and methods based on reconstructed object, camera positions, extracted 2D features, and so on have been proposed[3].

This research proposes an efficient noise removal method by clustering using the characteristics of object points and noise points when reconstructing an elongated object that spreads intricately in three-dimensional space, such as tree branches. The reconstruction point cloud has a partially different degree of density of points in the area. Because the noise point cloud tends to have a lower density than the object point cloud, noise is separated from the cluster. In this study, the optimum values of the parameters during clustering that enable separation were examined.

DBSCAN[4] was applied to clustering using the density of points. Since the number of points in the background is enormous and the calculation cost is high, the point cloud of the object was manually removed and clustered by dividing the point cloud into parts. Therefore, the parameters during clustering were determined by adapting to the characteristics of the tree branches. Noise could be identified by the proposed method, and the reconstruction point cloud of the object could be identified. In addition, it is considered possible to reconstruct the object surface by meshing the point cloud with noise removed.

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Effect of Shade on Optimal Placement Results of Photovoltaic Arrays

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Key Words: *Photovoltaic array*, *Placement optimization*, *Ray tracing*, *Genetic algorithm*, *Shade*

Photovoltaic arrays are installed on various shape sites to generate solar power on the ground. It is necessary to determine the arrangement of the PV array based on the influence of the solar orbit and shade to increase the amount of power generation. In order to maximize the amount of light received, the study was performed to optimize the placement of PV arrays based on the geographic data of the city[1]. Another study was conducted to determine the tilt and azimuth angles for PV arrays considering dust and maintenance space[2]. We proposed a method for finding the optimum placement of a large number of PV arrays in a site of arbitrary shape in a large-scale photovoltaic power generation facility[3].

The purpose of this study is to propose a method for analyzing shade generated in PV arrays and to clarify the effect of shade on the optimal placement results of PV arrays. An arbitrary placement in which multiple PV arrays are arranged independently on the site one by one is considered. First, the shaded area concerning the solar orbit and the array placement is formulated to estimate the decrease in the amount of light received by the shade. The area of shade on the PV array is obtained by dividing the surface of the array into triangular planes and tracing the rays obtained from the sun's orbit. An optimization problem in which the parameters are the tilted angle, azimuth angle, and placement position of the PV array is formulated. The placement is optimized to increase the amount of light received by installing multiple PV arrays at the site. A genetic algorithm is used for the optimization method.

Optimal solutions were found for some examples of optimal placement of each PV array on an arbitrary-shaped site. In the placement optimization, we compared and examined the placement results when and without considering the amount of light received due to shade and showed the effectiveness of arbitrary placement optimization considering the effects of shade.

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Hierarchal Polynomial Wavelet Decomposition for Full-Field Material Calibration

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Key Words: Full-field, Material Calibration, Inverse Problems, Polynomial Decomposition, Digital Image Correlation, Wavelets

Physics and engineering simulation tools are becoming more prevalent in decision making processes. Core to many engineering simulation tools is a series of material models that emulate the materials' physical responses. Traditional material model calibration consists of optimizing a material model against a limited set of probe data and homogenized boundary data. These traditional methods can calibrate a wide range of material models. However, as the complexity of the models increase, the number of experimental setups required to adequately calibrate the model increases as well.

Advances in experimental techniques have enabled the use of full-field kinematic and temperature data in material model calibrations. Full-field data capture has the potential to reduce the number of experiments required by capturing more complicated material evolutions in a single experiment, than captured by traditional experimental setups [1]. Full-field data can be difficult to work with because of dimensionality of the data set. Like other scientific data, full-field data often contains significant patterns. Patterned data is an attractive application for data compression. Compressing patterned data dramatically reduces the number necessary data points, while preserving the significant information present in the data.

In this talk I will present work on a hierarchal polynomial wavelet decomposition (HPWD) method for performing calibrations to full-field data. HPWD is an unstructured data compression method based on the concepts of tree wavelets [2] and polynomial field decomposition [3]. HPWD leverages the ability of tree wavelets to efficiently capture discontinuous material behavior, while preserving polynomial field decomposition's ability to compare compressed data across different realizations of the same domain.

Numerical optimization with HPWD uses a cost function defined by the differences in the most significant compressed data components. This formulation improves the cost function topography over traditional cost function definitions and provides the means for explicit feature emphasis. We will demonstrate these capabilities though one- and two-dimensional material calibration examples.

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Multi-objective optimization for minimizing weldline and cycle time using rapid heating cycle molding with heater system

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Key Words: *Plastic injection molding, Rapid heating cycle molding, Heater system, Engineering optimization, Optimum design*

Plastic injection molding (PIM) is a typical manufacturing technology to produce plastic products, and it is important to determine process parameters for high product quality and high productivity. The process parameters are conventionally determined by trial-and-error method through experiment, but computer aided engineering (CAE) is recently used as the alternative. Since the PIM simulation is computationally expensive, response surface approach is used to determine the optimal process parameters. Weldline that is formed when two or more melt plastic flow meets is one of the major defects, and it is preferable to reduce the weldline as much as possible for the surface quality and strength of plastic products. Rapid heating cycle molding (RHCM) that the mold temperature is actively controlled has been recognized as an innovative PIM technology for weldline reduction. By heating up the mold temperature, the melt plastic is smoothly flowed into the die cavity, and consequently the weldline is well reduced. To quickly heat up the mold temperature[1], a heater system is newly introduced in the RHCM. Many papers using the RHCM discuss on the weldline reduction, but the process parameters as well as the mold temperature profile is rarely discussed. In this paper, the process parameters in the RHCM using heater system are optimized. A multi-objective optimization for minimizing both weldline and cycle time is considered, and then the process parameters as well as the mold temperature profile is determined. Sequential approximate optimization that the response surface is repeatedly constructed and optimized is adopted for the design optimization[2], and the pareto-frontier is identified. Based on the numerical result, the experiment using PIM machine (MS100, Sodick) is also conducted to examine the validity of the RHCM with heater system.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Performance Evaluation of a Plate-fin Heat Exchanger Core Designed Using Localized Topology Optimization

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Key Words: Heat Exchange, Topology Optimization, CFD Analysis, Additive Manufacturing, Design Process

Plate-fin heat exchangers are a common type of heat exchangers often selected for their compact and lightweight designs. The flow paths of two fluids exchanging heat are separated by plates and interchangeably stacked on top of each other. Within the flow paths, the two plates are connected by fins whose design depends on the targeted performance for the heat exchanger. This design is simple and repetitive resulting in a exchanger core with a very fine internal structure that is compact and lightweight.

With the recent advances in topology optimization for fluid and thermal-fluid problems, potential improvements to heat exchanger design have been considered. However, obtaining a full heat exchanger design, by means of topology optimization, that would have the similar or better performance to conventional designs, is not feasible due to extreme computational costs associated with such an optimization analysis. Therefore, the natural approach is to constrain the optimization to a small section of the heat exchanger and extrapolate the heat exchanger design from that section.

In this study, we deploy a Level-set based topology optimization method for a thermal-fluid problem in two dimensions to obtained optimized fin cross-sections. The use of 2D optimization allows for quick generation of a relatively complex topology as opposed to 3D optimization. The resulting optimized topology shows repetitive internal sections indicating potential for more localized optimization to even higher degrees of complexity. The derived 2D cross-sections are gradually extended to small 3D sections, full flow paths, and finally the full core, with design performance evaluated at every step. To eliminate the need for costly computational fluid dynamics (CFD) analysis to obtain the performance values of the whole heat exchanger, we develop a methodology for performance evaluation of the whole design based on the performance of the single optimized section. As a result, we show that the evaluated performance is in good agreement with numerically and experimentally obtained performance values for the whole heat exchanger core.

Prediction for Behavior of Underground Structures during Construction Phase Using Data Assimilation

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Key Words: *ensemble-based data assimilation, underground structures, code verification*

To ensure safety during the construction phases of underground structures, the present and future conditions of the rock and tunnel supports such as displacements and stresses, must be estimated and predicted by appropriate measurements and numerical simulations. However, many uncertainties, e.g., geological structures, mechanical properties of rocks, initial and boundary conditions, complicate numerical modelling considerably.

To solve this problem, the research developed a numerical analysis system using a data assimilation (DA) technique, that updates the numerical model based on measured data during construction. In this system, a finite volume method is applied to solve partial differential equations of rock mechanics. The Error Subspace Transform Kalman Filter is used for the DA.

To evaluate the effectiveness of the proposed system, numerical experiments were performed for a simple linear elastic problem of excavating an unsupported circular tunnel. The excavation behavior of the tunnel to be predicted was also calculated by a similar numerical analysis, instead of using the measured data of an actual tunnel. This surrogate tunnel excavation problem was adopted as subject to verification, which can be accurately predicted using this system.

The state vector included Young's modulus, E, and the displacements of the rock. The model state was sequentially updated by the system which assimilates the observed displacements using a 50-member ensemble. Observation points were established at the crown and side walls of the tunnel cross-section. The synthetic tests were performed in three ways. The first was in accordance with the general scheme of sequential DA that the latest updated ensemble was used in the next excavation stage. In the second, only the latest updated Young's modulus, E^a, was used in the next excavation stage. In the last one, E^a was introduced into initial model before excavation and then excavation analyses were performed again.

It was found that the behavior of the rock could not be predicted correctly under the conditions of this verification problem unless the latest updated E^a is introduced into initial model before excavation and the excavation analyses are redone from this stage.

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Stacking Sequence Optimization for Ply Drop-off Laminated Composite Considering Some Empirical Constraints

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Key Words: Stacking Sequence Optimization, Ply Drop-off Laminate, Empirical Constraints, Strength

This study addresses the stacking sequence optimization of the tapering laminated composite consisting of 0°, $\pm 45^\circ$ and 90° plies with ply drop-off considering the empirical constraint conditions. The stacking sequence of the thin-side laminate is determined in advance, while for the thick side, only the ply thickness ratio and the surface plies are determined in advance as the reinforcement design conditions. Then, the stacking sequence of the thick side and the order of ply drop-off are designed to maximize the strength in the ply drop-off region under following constraints. All plies of the thin-side laminate should be continued to the thick-side, the cover and the second layers should not be dropped off, and the adjacent plies should not be continuously dropped off. In addition, the allowable number of contiguous plies, the allowable orientation angle difference between neighboring plies are considered as empirical constraints. The optimization problem with these empirical constraints is solved by using genetic algorithm with our proposed genetic operators [1]. The strength criteria is evaluated at the resin pocket by using the FEM model of the tapered three-ply laminates that the middle layer is dropped off [2]. For the efficient optimization procedure, the look-up table for the strength criteria consisting of all possible combinations of the three-ply laminates is prepared in advance from the FEM analysis and just called during the optimization run [3]. Through numerical examples, the optimum designs for some kinds of tapered laminates from 48 to 24-ply tapered laminates under several conditions are evaluated. Then, validity of the proposed optimization method is discussed.

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Topology optimization based on level set method of potential problems for general nonlinear boundary conditions

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Key Words: Galvanic Corrosion, Nonlinear Boundary Conditions, Topology Optimization, Level Set Method, FreeFEM++

Optimization problems in thermal, structural, electrostatic and other fields governed by Laplace's and/or Poisson's equations are important in various engineering design applications. In particular, level-set based topology optimization is one of the strong approaches for solving the field shape design problems, in which the shape of the material or field is related to a distribution of a scalar function of point called level set function. From the distribution of the level set function, the boundary and the material/field domain are extracted. By updating iteratively the distribution of the level set function that satisfies a reaction-diffusion equation with a source term related to the sensitivity of the objective functional, the optimum arrangement of the material/field is obtained.

In the topology optimization problems governed by Laplace's or Poisson's equations, linear boundary conditions have usually been assumed [1]. However, there exist a class of problems in which nonlinear boundary conditions have to be considered even if the governing equation is linear, such as galvanic corrosion [2] and thermal radiation problems. In this study, we consider a topology optimization using the level-set method for a problem with arbitrary nonlinear boundary conditions. Topological derivative is derived for an objective functional under the nonlinear flux boundary condition. The finite element method software FreeFEM++ is used for calculating the topological derivative values and the numerical scheme of the topology optimization using FreeFEM++ is shown. Some numerical examples are also shown to demonstrate the present formulation.

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Topology Optimization of Magnetic Circuit Geometry in Thermomagnetic Motors

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Key Words: *Coupled analysis, Magnetic field, Thermo-magnetic motor, Power, Temperature-sensitive magnetic material, Magnetic Circuit, Topology Optimization.*

A thermomagnetic motor[1], [2] can generate torque by changing the magnetic distribution generated by permanent magnets by heating and cooling temperature-sensitive magnetic materials[3]. Therefore, thermomagnetic motors have the potential to extract mechanical energy from hot water below 100 ° C. One of the problems with this motor is that it has not reached the stage of practical use due to its low output[1], [2].

The thermomagnetic motor proposed by the authors[2],[4] is cylindrical. Permanent magnets and yokes are located on the motor's stator, and the rotor is made of a temperature-sensitive magnetic material. Using hot and cold water to heat and cool the area between the rotor and the stator creates a temperature distribution in the temperature-sensitive magnetic material, giving it magnetic saliency. This structure does not have the flux barrier used in standard PM motors. The short circuit of the magnetic flux from the permanent magnets is large, so it is thought that sufficient rotational torque cannot be generated.

In this study, the shape of the stator region around the permanent magnet is optimized to increase the output. As a result of topology optimization, air regions that function as a flux barrier are created around the permanent magnet, and the rotational torque is improved.

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Toward Concurrent Multiscale Topology Optimization for High Heat Conductive and Light Weight Structure

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Key Words: *Concurrent topology optimization, Heat conductvity, homogenization method, periodic microstructure.*

In several disciplines of engineering, high heat conductive solid structures of lightweight solid structures play a significant role. Due to advancements in computer-aided design and quick growth in additive manufacturing, topology optimization uses in designing high heat conductive structures has grown significantly in recent decades and remains a very appealing issue to be tackled. However, achieving optimal high conductive structure with utilizing topology optimization is a challenging task such that, it is quite sensitive to optimization factors such as the searching step and initial conditions. In this work, an investigation of maximizing heat conductivity with minimizing weight is conducted, with adopting heat compliance minimization as the objective function. The optimization first addressed the macro scale point of view of the structure, by investigating the optimization parameter's effect on the performance of the optimized resulted structure. Furthermore, we extended the examination toward multiscale topology optimization to achieve excessive light-weighting of heat-conductive structures. During the concurrent optimization process, the numerical homogenization approach was utilized to compute the effective heat conductivity of the microstructure and concurrently updating the macrostructure system. As a result, the periodic boundary conditions are simulated on a microscale with a dedicated finite element model, while the effective characteristics are implemented on a macroscale. the suggested design methodology of this work in several examples which showed good responses of the microscale design for the macroscale design domain boundaries conditions. This response is shown through the varied designs of multiple examples of different boundary conditions. This research showed that, utilizing weight reduction with considering the total volume reduction on macro and microscale gave better performance compared to limited the weight minimization on the macroscale alone. The volume-to-point approach was successfully expressed for the macroscale design by obtaining the micro channeling of the conductive material for the macro design domain, which is associated with better performance than single microstructure concurrent optimization, according to the studied cases of optimizing multiple micro design domains. This is because the increased freedom of attaining robust design variable distribution on both the microscale and macroscale allows for this.

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Unit Cell Design of Fatigue-tolerant Lattice Structures for Bone Implants

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Key Words: *Lattice Structures, Design, Fatigue-tolerant, Bone implants*

The porous design of bone substitutes not only promotes bone ingrowth but also plays an essential role in facilitating vascularization as well as nutrition and waste transportation [1]. The current designs of lattice structures for bone implants mainly focus on matching the elastic modulus with the natural bone to alleviate stress shielding [2]. However, fatigue failure contributes to most of the structural breakdown even when the structure is subjected to elastic deformation under cyclic loading, which is seldom considered in lattice unit cell design. This paper presents design of fatigue tolerant lattice structures while maintaining sufficient mechanical strength using PolyStress [3]. The optimization problem model is constructed according to the work condition of hip bone implants. The fatigue strength of the design is realised by stress constraints and the elastic modulus is controlled by a stiffness constraint. The unit cell is periodically designed and several boundary conditions are considered. Compared to the traditional CAD and Triple Periodic Minimal Surface (TPMS) design of lattice structures, this newly proposed method provides unit cell topology based on its application requirements, such as the fatigue life which is beneficial to extend bone implants' service life. In addition, introducing topology optimization into the design phase creates lightweight structures and saves materials for manufacturing.

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A R&D software platform for shape and topology optimization using body-fitted meshes

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Key Words: topology optimization, level set method, adaptive remeshing

Topology optimization is devoted to the optimal design of structures. It aims at finding the best material distribution inside a working domain while fulfilling mechanical, geometrical and manufacturing specifications. The need for lighter and efficient structural solutions has made topology optimization a vigorous research field in both academic and industrial structural engineering communities. This contribution focuses on PISCO, a Research and Development software platform for shape and topology optimization where the computational process is carried out in a level set framework combined with a body-fitted approach [3]. The level set method relies on the classical sensitivity analysis from the shape optimization framework to compute a descent direction and advect the structural interface. In the present setting the level set method is coupled with a remeshing routine which enables the reconstruction of a body-fitted mesh at each step of the underlying optimization process, as proposed in [1, 2]. Since the structural interface is known explicitely at each step of the iterative procedure, the body-fitted approach simplifies the evaluation of the mechanical quantities of interest. PISCO is composed of several components including an algorithmic toolbox specialized in the treatment of level sets, a generic interface to finite element solvers, a toolbox handling mesh files in several classical formats, several algorithms for the resolution of constrained optimization problems, physical and geometrical optimization criteria and an advanced interface to the remeshing tool mmg3d. The components devoted to the physical analysis computations and the constrained optimization algorithms are implemented in a generic fashion in dedicated modules. The non-intrusiveness of the implementation is proved by the coupling with several external physical solvers. We rely on a gradient-flow numerical optimization algorithm to handle the balancing between the minimization of the objective and the non-violation of the constraints. Several industrial applications are presented to highlight the capabilities of the platform.

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Accelerated Projected Gradient Method for Topology Optimization of Heat Conduction Problem

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Key Words: Topology optimization, heat conduction problem, optimization algorithm, accelerated gradient method

Topology optimization problems are often large-scale. Therefore, a fast optimization algorithm that can solve a large-scale optimization problem in practical time is demanded. In our study, we extend the accelerated projected gradient method [1], which was originally developed for solving the compliance minimization problem, to the heat conduction problem.

Accelerated gradient methods have been actively studied in the machine learning community in recent years. They are first-order optimization algorithms which only use the first derivatives (gradients) of the objective function, but the convergence rate is improved compared to the conventional gradient descent method. As the iteration cost of first-order methods is very cheap compared to second-order methods (e.g. the sequential quadratic programming), first-order methods are more suited for large-scale optimization problems. Accelerated gradient methods were originally developed for convex optimization. Recently, such acceleration techniques have been extended to nonconvex optimization problems.

As many topology optimization problems are large-scale and nonconvex, accelerated gradient methods can be suitable for topology optimization. In our study, we consider the heat conduction problems with simple linear constraints so that we can use the projected gradient method. The projected gradient method is a classical way to solve a constrained optimization problem, using the projection onto the convex feasible set. We show that, in our problems, the projection onto the feasible set can be easily calculated by a bisection method both for the equality and inequality constraints on the volume. To accelerate the convergence, we use the acceleration technique by Ghadimi and Lan [2] and the heuristic stepsize policy [1] considering properties of topology optimization problems. Moreover, the proposed method is easy to implement. We conduct several numerical experiments to compare the performance of the proposed method with the existing methods (e.g. the optimality criteria method and the method of moving asymptotes). It is demonstrated that the proposed method converges faster, especially when the number of finite elements is large. We also discuss a condition under which the convergence is guaranteed.

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Adaptive mesh refinement in level set based body-fitted topology optimization

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Key Words: topology optimization, level set method, adaptive remeshing, anisotropic remeshing

Topology optimization is devoted to the optimal design of structures. It aims at finding the best material distribution inside a working domain in order to satisfy mechanical, geometrical or manufacturing specifications. The need for lighter and efficient structural solutions has made topology optimization a vigorous research field in both academic and industrial structural engineering communities. In the present setting the level set method is coupled with a remeshing routine which enables the reconstruction of a body-fitted mesh at each step of the underlying optimization process, as proposed in [1, 2]. Since the structural interface is known explicitely at each step of the iterative procedure, the body-fitted approach simplifies the evaluation of the mechanical quantities of interest. The body-fitted remeshing strategy proposed in [1, 2] is driven by global user-defined parameters such as the minimal/maximal mesh size or the gradation of the desired mesh. In this contribution we propose to couple the body-fitted approach with adaptative remeshing techniques involving an anisotropic recovery-based a posteriori error analysis. The gradient-recovery Zienkiewicz-Zhu-type error estimator developed in [4, 5] is applied to drive isotropic or anisotropic mesh adaptation at each step of the underlying optimization process. The proposed error estimator is used from one hand to control the accuracy of the discretization of the structural interface, from the other hand to control the discretization error linked to the numerical evaluation of mechanical criteria and sensitivities in order to speed up the overall optimization routine. All the proposed numerical examples are realized using PISCO, a Research and Development software platform for shape and topology optimization in active development at IRT SystemX. We rely on a gradient-flow optimization algorithm designed to decrease both the value of the objective function and the violation of the constraints. Several industrial-related applications are presented to illustrate the capabilities of the proposed method.

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Applications of the Model Order Reduction Using Variational Autoencoder to PDE-Constrained Topology Optimisations

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Key Words: Topology Optimisation, Variational Auto-Encoder, Data-driven, Model Reduction

In (PDE-constrained) structural optimisations, it is interesting and challenging to take account of "human-oriented design" because an optimisation emphasises to realise a certain functionality rather than design/outlook/form of a target object. In addition, designs made by human would be provided as sketches rather than mathematically-defined geometries, in particular, when the designs are artistic. Then, it is not easy to handle such pictures numerically. To overcome these two difficulties, Guo et al [1] proposed a framework based on Variational Auto-Encoder (VAE). The VAE enables to create an arbitrary dimension of latent variables to change the shape of a target over given designs almost continuously, although the meaning (e.g., length, angle, curvature) of the latent variables are ambiguous. Once latent variables are obtained, one can perform a structural optimisation by using latent variables as design variables in a certain optimisation method. Guo et al [1] applied their data-driven and dimension-reduced framework to a 2D heat conducting design problem with the help of the genetic algorithm.

Following Guo et al. [1], we apply their framework to a minimisation problem of the mean compliance of a 2D linear elastic body as well as a maximisation problem of the sound pressure at an observation point for 2D acoustics. To solve those problems, we first prepare several pixel data and parameterise them by some latent variables. Then, we exploit a gradient-free non-linear optimisation method (such as the COBYLA method) to minimise/maximise the objective function with respect to the latent variables. Regarding the compliance problem, we could obtain the optimised solution, which resembles to given designs. The result of the acoustic problem will be mentioned in our talk.

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AuTONR: Topology Optimization via Neural Representation and Automatic Differentiation

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Key Words: Topology Optimization, Neural Network, Reparameterization, Automatic Differentiation

The rapid development of deep learning has brought new opportunities for the exploration of topology optimization methods. The combination of deep learning and topology optimization has become one of the hottest research fields at the moment. In this work, the neural network is directly used for topology optimization. The update of the design variables (pseudo-density) in the conventional topology optimization method is transformed into the update of the neural network's parameters, which is called *Neural Reparameterization*. The sensitivity analysis in the conventional topology optimization method is realized by the powerful *Automatic Differentiation* technology. We verify the effectiveness of AuTONR on various numerical examples, including the stiffness optimization problems, the stress-constrained problem, structural natural frequency optimization problems, compliant mechanism design problems, heat conduction system design problems. Compared with the existing methods that combine deep learning with topology optimization, AuTONR does not need to construct a dataset in advance and does not suffer from structural disconnection. The structures obtained by AuTONR can be comparable to the conventional methods.

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Basic study on PDE-based thickness constraint of topology optimization

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Key Words: Topology optimization, Geometrical shape feature, Thickness

Thickness constraint is quite important for the structural optimization method, especially for topology optimization. Thickness control is needed for many kinds of molding processes, such as injection molding. Many studies have been conducted on the thickness constraint [1], but most of them are based on a distance function or other time-consuming methods. Since the approach using distance function is an indirect way to consider the thickness, these formulations tend to become complex.

We present an approach for the thickness constraint based on the Fictitious Physical Model (FPM). The FPM is introduced to evaluate geometric features as if they were physical phenomena expressed by the partial differential equations. The FPM is formulated as a linear partial differential equation system. The approximated local thickness is defined based on the solution of the PDE. The thickness constraint is formulated using the local thickness, and its design sensitivity can be derived based on the adjoint variable method.

The main advantages of this method are its simplicity of formulation and its computational cost when calculating the thickness. In addition, it can directly evaluate a kind of thickness, and the thickness constraint can be handled much easier than the previous methods. For example, this method may be applied to maintain the thickness constant whole design domain.

In this research, we propose a level set-based topology optimization method for thickness control. First, the definition of the local thickness is explained. Then, numerical examples are given to confirm the validity of the local thickness. Finally, the topology optimization problem with a thickness constraint is formulated and several optimized designs are provided.

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Derivation of effective permittivity using machine learning and its application to collimator design

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Key Words: *Topology Optimization, Composite, Electric Permittivity, RVE method, Deep Learning, Collimator*

Nowadays, composite materials, which is a material that consists of various distinct constituents or phases, play an important role in aerospace and structural engineering applications. As the need for numerical implementation increases in the design of structures made of composite materials, methods for effectively deriving material properties and designing structures have been sought. With respect to these issues, we present the derivation of the effective permittivity of an anisotropic composite material based on a representative volume element method (RVE) [1,2] and machine learning (ML) [3]. After calculating the effective electrical permittivity of the anisotropic composite, ML models based on DNNs with multiple layers are used to build the continuous functions of the effective properties. With the regression function from ML, we can handle the electrical permittivity at each node point. It is noteworthy to reflect the anisotropic composite material easily in the optimization design process. Here, we conduct numerical example about a dielectric collimator design using the ML model to verify the proposed method. The finite element analysis for solving the electromagnetic wave problems in optimization procedure and conducting the RVE method were performed by using the commercial package COMSOL. The ML and the optimization process were programmed using the Matlab programming.

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Design of Channels under Turbulent Subsonic Compressible Flow Using Topology Optimization

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Key Words: *Topology optimization, turbulent flow, compressible fluid, subsonic flow.*

Topology optimization (T.O.) under compressible turbulent flow regime is still an open problem due to CFD challenges related to viscosity variation, shock waves, and compressibility factors that hinder the simulation and its adjoint model hand derivation. One work has been developed at laminar compressible regime [7] but turbulence has been treated only at incompressible flow [2][3][4][6][8]. Therefore, in this work we propose a T.O. formulation for compressible turbulent subsonic flow regime (0.3<Mach<0.7) aiming to minimize the energy dissipation. Also, turbulence is modelled by means of the Favre Averaged Navier-Stokes (FANS) equations and the Spalart-Allmaras turbulence model in a steady-state regime considering ideal-perfect gas model, and isothermal wall boundaries. The adjoint model is obtained with an automatic differentiation tool [5] that avoids hand derivation, and the internal point optimizer (IPOPT) solves the optimization problem. The primal model is solved in a finite volume method (FVM) based-software, and the adjoint model in a finite element method (FEM) based-software, which are linked in the authors' developed platform "FEniCS TopOpt Foam" [1]. Different 2D cases at compressible subsonic turbulent regime are optimized and energy dissipation is compared with baseline designs. The method is robust and flexible, establishing a first step in T.O. of the compressible turbulent regime.

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Design of large displacement compliant airfoil through stress constrained topology optimization

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Key Words: *Stress-based topology optimization, morphing wings, compliant mechanisms, large displacements*

The present work investigates the design of a flexible mechanism for compliant airfoils by means of topology optimization. Compliant airfoils consists in a form of morphing concept for wings, which have been developed in recent years, aiming to reduce weight and maintenance costs, among other advantages. One way of obtaining the morphing structure is by designing a mechanism that does not have multiple separate parts connected by conventional hinges with bearings. Here, a nonlinear approach for topology optimization is considered, where the displacement of the profile trailing edge is maximized under volume and global stress constraints. The static equilibrium is obtained via a nonlinear finite element approach, with a hyperelastic material model. The method is applied to an asymmetric airfoil, where the area behind the half chord point is the design domain. A concentrated force is applied in the horizontal direction and the vertical displacement of the trailing edge is maximized, with a prescribed volume fraction of the initial design domain. The work investigates different stress limits, as well as the effect of neighbor radius and input forces. Optimized designs are obtained, resulting in efficient single compliant airfoils, respecting given constraints.

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FFT-based Multi-scale Topology Optimization with High-resolution Microstructure

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Key Words: Multi-scale Topology Optimization, Fast Fourier Transform, Homogenization Method

Thanks to the development of additive manufacturing (AM) technology, it is becoming possible to produce materials with desired mechanical properties defined by their periodic microstructures. To design optimal microstructures, multi-scale topology optimization (MTO) has been paid attention to in many engineering fields.

As an example of MTO, Kato et al. [1] proposed an analytical sensitivity analysis with an adjoint method based on a decoupling scheme [2]. This method with a simple algorithm has reduced computational cost and made MTO more feasible compared with the previous methods. However, compute time and memory requirements are still high, and these prevent practical use such as high-resolution 3D analysis for precision modeling with AM and non-linear analysis assuming actual materials.

In the above method, finite element method (FEM) is used to analyze periodic microstructures, but this research focused on an alternative approach using fast Fourier transform (FFT) by Moulinec and Suquet [3]. This FFT-based homogenization adopts simple point-wise discretization and is known as an efficient method to analyze periodic microstructures. Therefore, the application of this method to the microstructural analysis of MTO can be expected to reduce computational costs.

In this study, as a basic problem, we mainly deal with topology optimization of microstructure for maximizing linear stiffness of macrostructure. First, by comparing obtained topology and objective function values, we demonstrate that the proposed method with FFT can accurately compute and obtain almost the same result as the conventional method with FEM. Then, by measuring relations between mesh resolution and computational cost, we reveal that the proposed method can compute faster with lower memory usage, especially for 3D analysis.

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Including Anisotropy of Additively Manufactured Bulk Materials in Topology-Optimized Designs

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Key Words: *Topology Optimization, Additive Manufacturing, Anisotropy*

The recent rapid development of Additive Manufacturing (AM) technologies has created a need for new design methods that can leverage the new, increasingly complex fabrication possibilities. Topology optimization is frequently suggested as a powerful design-for-AM approach because it does not require a preconceived notion of the final structural layout. Therefore, the past decade has seen a significant research interest in tailoring topology-optimized design to AM. Examples include the considerations of overhang constraints, infill design and enabling design with multiple base materials. However, the anisotropic bulk material behavior associated an array of AM processes has received less attention. The anisotropy can develop (even when using isotropic base materials) as a consequence of the weak bonds along the print path and layer-by-layer fabrication process. This works seeks to address the anisotropy of bulk AM materials in topology-optimized design in two ways; both globally and locally.

Considering a globally anisotropic bulk material, this work experimentally investigates the effect of assumptions of isotropy versus anisotropy within the design framework. All test specimens are prepared using Fused Filament Fabrication (FFF). Topology-optimized designs are obtained for simply supported beams with a range of different volume fractions. A density-based approach [1] is used and the Method of Moving Asymptotes is taken as the gradient based optimizer [2]. The experimental behavior of the samples with assumptions of isotropy and anisotropy (in different directions) is evaluated and compared.

In addition, this work considers the local anisotropy induced in most material extrusion AM processes. Material extrusion here refers to technologies where a nozzle moves across a 2D slide of the design and deposits material. Based on the previous work by the authors [3], we propose a novel topology optimization algorithm which seeks to capture the local anisotropic behavior by mincing the material deposition process. This is done using modified Discrete Object Projection [4] with two distinct base materials; i) a stiff core, and ii) a more compliant bonding region. The algorithm is demonstrated on benchmark minimum compliance problems.

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Inverse Design of Thermal Conductivity Tensor based on Free Material Optimization

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Key Words: Free material optimization, Heat conduction, Second-order constitutive tensor

Free Material Optimization (FMO) [1] is a structural optimization method that encompasses the design of structural materials in a broad sense, where the elements of the constitutive tensor are the design variables. When restricted to the microstructure composed of isotropic materials, the material properties can be expressed as a set of semi-positive definite symmetric constitutive tensors. This approach has been used to generate tape layup procedures for composite materials and to design local microstructures that achieve the targeted elastic tensor properties [2]. Removing the restriction of symmetry of the constitutive tensor would further extend the design space and improve the theoretical performance limit of devices, but it is not clear whether such materials exist in reality. On the other hand, it has been reported that the symmetry of this constitutive tensor can be apparently broken by combining it with other physical phenomena without closing it to a single physical phenomenon. Such a situation justifies extending the space of the constitutive tensor to an asymmetric domain, but it is necessary to deal with new constraints, such as to what extent the asymmetry should be allowed. In this study, we consider a topology optimization method with asymmetric constitutive tensors as design variables in the case of second-order constitutive tensors using the heat conduction problem as an example. Several numerical experiments will be provided in the presentation to show the validity and the utility of the design of an asymmetric constitution tensor.

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Large-Scale Topology Optimization of Unsteady Incompressible Flow with Building-Cube Method

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Key Words: Topology optimization, Finite volume method, Parallel computing, Unsteady flow

Topology optimization methods have been adopted for not only structural problems but fluid problems in recent years. Although almost all topology optimization methods for fluid problems assume steady-state flows, Deng et al. [1] proposed a topology optimization method for unsteady flow by adding the artificial Darcy frictional force into the incompressible Navier-Stokes equations. The optimization procedure is implemented using the continuous adjoint method and the finite element method. However, the topology optimization of unsteady flows requires a high computational cost because the fine mesh is indispensable, especially for high Reynolds number flow.

Considering the background mentioned above, we propose an unsteady flow topology optimization method using the cell-centered finite volume method with the building-cube method (BCM) [2][3][4], which is suitable for massively parallel computing. In the BCM, the computational domain is divided into cubic regions called cubes. Each cube is divided at equal intervals, the same number of cubes is assigned to each core, and the spatial loop processing is executed for each cube. The sensitivity of the objective function is obtained by continuous sensitivity analysis based on the adjoint variable method for the topology optimization procedure. In the presentation, we will demonstrate several numerical examples to verify the proposed method.

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Level set-based topology optimization for sound-absorbing structures including thermal and viscous boundary layer effects

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Key Words: *Acoustics, Boundary layer effects, Sound absorption, Topology optimization*

In this research, we conduct topology optimization for sound-absorbing structures that efficiently absorb noises within a certain frequency range with a consideration of thermal and viscous boundary layer effects.

Acoustic devices that control the behavior of acoustic waves have been widely used in our daily life, represented by noise barriers and music instruments, etc. There have been a variety of acoustic devices over different scales proposed, and miniaturization of them is one of the hot topics in acoustics. Acoustic metamaterial [1] is a typical structure that drastically controls waves with a tiny structure much smaller than the wavelength. The functions of these acoustic devices strongly depend on their structural design, and topology optimization [2] has been introduced for them to achieve the desired performance.

In such a tiny structure, acoustic waves propagating in air-filled channels are affected by the thermal and viscous boundary layers, which are present in the vicinity of the solid surface. The behavior of waves is quite different from that in bulk due to the damping by these layers. Therefore, consideration of these boundary layer effects is essential for the design of acoustic devices that possesses tiny channels.

We propose a level set-based topology optimization method for acoustic devices with air-filled channels with the consideration of thermal and viscous boundary layers and apply the method to the design of sound-absorbing structures.A sequential linearized Navier—Stokes model [3] is introduced to model the boundary layer effects. The design sensitivity is approximately derived based on the concept of the topological derivative. Several numerical examples of sound-absorbing structures are provided using the level set-based topology optimization method and they show the validity and utility of the proposed method.

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Level-set based topology optimization of a microfluidic mixing problem

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Key Words: Static Mixer, Level–set Method, Fluid Topology Optimization, Mesh Adaptation, Parallel Computing, FreeFEM-PETSc-Mmg

Static mixers are widely used in chemical industry such as gas mixing, wastewater treatment process and chemical reaction. The major concern of the static mixer from an engineering perspective is to achieve a better mixing efficient under a lower power dissipation. Therefore, we propose a topology optimization(TO) method for static mixer based on level-set method. We use reaction–diffusion equation for updating the level set function which can explicitly describe the boundaries between different material phases. We calculate the two– and three–dimensional test cases. Three remarkable key points are highlighted here: (i) we introduce a body-fitted mesh adaptation technique. The body fitted mesh relies on a third-party package Mmg; (ii) we formulate the optimum design problem for maximization of mixing and use the continuous adjoint method to derive the sensitivity. Moreover, we validate the deduced sensitivity by comparing it with a finite difference results; (iii) FreeFEM is used for finite element analysis and PETSc for parallel computing. Several benchmark numerical examples are presented to support these remarkable features.

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Mechanism Synthesis of 1-DOF Transformable Wheel Structure Based on Kinematic Simulation and Topology Optimization Method

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Key Words: *Mechanism design, Transformable wheel, Topology optimization, Forward kinematics-based simulation*

A transformable wheel mechanism efficiently moves in a circular state on flat ground and adaptively overcomes obstacles by modifying the shape of the wheel when it encounters various-sized obstacles [1]. So far, the adaptive motion was mainly generated by multi degree-of-freedom (DOF) mechanisms [2]. However, the operating cost of the multi-DOF mechanism is high because of structural complexity and many actuators. To overcome this limitation, we propose designing a 1-DOF wheel mechanism generating adaptive motion. However, it is complicated to identify a climbing strategy based on 1-DOF motion, and it is further challenging to synthesize 1-DOF mechanism that satisfies the target kinematics because there are no mechanism candidates based on the adaptive climbing strategy. Here, we 1) present a forward kinematics-based simulation model to establish adaptive wheel-climbing strategies and 2) propose a topology optimization method for synthesizing mechanisms that generates the target kinematics so that the wheel structure can successfully climb indoor-sized steps. First, a kinematic analysis model was developed to identify the target movement of the end-effector of the wheel to climb obstacles of various heights. Then, we propose a topology optimization-based synthesis method for 1-DOF transformable wheel mechanism to autonomously design the wheel structure. For the synthesis, we employ the topology optimization ground structure model which consists of zero-length springs and rigid blocks, called the JBM (joint-element connection rigid block model) because the model allows us to find an appropriate mechanism without starting with any baseline candidate mechanism [3]. Besides, for reducing complexity, we design the joint composition of the planar linkage mechanism by taking advantage of springs and blocks-based ground structure model. By using the developed method, novel transformable wheel mechanisms were successfully synthesized, and the kinematic and configuration characteristics of the designed mechanisms were investigated.

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Multi–material topology optimization of an eigenfrequency problem

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Key Words: Multi–material Level–set Method, Eigenfrequency Topology Optimization, Parallel Computing, Mesh Adaptation

We propose a novel framework for the multi–material topology optimization (MMTO) of an eigenfrequency problem. From the theoretical perspective, two key ingredients are highlighted: (i) multi–material level set (MMLS) method is constructed. With this method, the interfaces between different material phases are represented by the iso-surfaces of multiple level set functions. Hence, the optimal solutions have binary structure and they are free from greyscale elements; (ii) The proposed design methodology uses a reaction-diffusion equation (RDE) for updating the level–set functions based on the topological derivative, making it possible to nucleate new holes during optimization process. From a numerical standpoint, our framework uses FreeFEM for finite element analysis (FEA) and PETSc for distributed linear algebra. Efficient preconditioner techniques enable us to solve the large-scale finite element systems. The performance of our methodology is demonstrated by showcasing two– and three–dimensional benchmark test cases.

Multiscale Topology Optimization of Buckling-resistant Structures

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Key Words: *Multiscale design, Inverse homogenization, Buckling design, Stress analysis*

Multi-scale structures, achieving extreme and tuneable performances while being lightweight, are gaining increasingly more interest. For example, lattice materials and infilled structures have already proven to be more competitive than classical, single-scale, composites for some automotive and aerospace applications. On the other hand, the multiscale idea has recently gained popularity as a computational tool speeding up structural topology optimization. Stiffness optimized designs consisting of millions of design variables have been obtained at a remarkably low computational cost, by coupling traditional homogenization-based topology optimization with a de-homogenization step interpreting the optimized set of material properties with a single-scale structure [1].

Extending this method to the design of buckling resistant structures is the topic of this work. To do this, difficulties arising when including buckling in the analysis and design of multiscale structures must be overcome. First, analytical solutions and theoretical bounds are not known for the buckling response, and the optimized unit cells must be found numerically. Second, such unit cells show a high dependence on the stress state, making very complicate to achieve a stable design under multiple load conditions [2]. Finally, the de-homogenization is made challenging by the presence of many simultaneous, local buckling modes [3] and stress concentrations, potentially disrupting the performance of the infill.

A thorough analysis of the origins and effects of these issues is given, possible remedies are discussed, and multiscale designs optimized for extreme buckling resistance are shown.

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Noble Design of Adaptive and Efficient Knee Exoskeletons by Mechanism Topology Optimization Method

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Key Words: *Topology optimization of linkage mechanism, Knee exoskeleton, Self-alignment*

Knee joint exoskeletons play a critical role in assisting the movement of disabled and non-disabled humans. These wearable knee exoskeletons should generate sophisticated movement due to rather complicated knee joint motions and also interact safely with their wearers. Therefore, the designed knee exoskeletons should be adaptive to make them universally useful for humans of different body shapes [1]. Lightweight and cost-effectiveness are also other design considerations for the knee exoskeletons. However, because of several design requirements to consider, it is difficult or sometimes impossible to devise such knee exoskeletons even with many trials and errors. To overcome these difficulties, we present a novel design method to synthesize self-aligning and actuation-efficient knee exoskeleton mechanisms without any baseline design, a method similar to the structural topology optimization method.

The knee exoskeleton mechanism to be designed here is not just supposed to follow a specific path but to generate a desired knee instant center of rotation workspace. Furthermore, it should possess self-aligning capability by which undesirable force should not be applied to the human joint and also possibly yield the desired profile of mechanical advantage during gait motion. Here, we employ the ground model applied to the mechanism topology optimization method [2-3], which can represent any two-dimensional linkage mechanism possibly consisting of rigid links and revolute and prismatic joints. Moreover, we develop a new optimization-based formulation to achieve our design objectives. A few numerical results that validate our approach will be presented, along with a fabricated 3D-printed mock-up. Finally, the simulated actuation torque-speed curve using the designed exoskeleton confirms that the synthesized mechanism is safe and comfortable to wear and requires relatively low-powered actuation.

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Optimization-based synthesis of 1-DOF underactuated spring-linkage mechanism

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Key Words: *Underactuated Linkage Mechanism, Spring-linkage mechanism, Adaptive Mechanism, Path Generation Synthesis Problem, Automation Mechanism Synthesis Method.*

For a mechanism to be adaptive in a two-dimensional plane, it must have more than one-degree-of-freedom (DOF). For example, a 1-DOF fully actuated mechanism having a single actuator can only follow a specific path. On the other hand, a single actuator-driven 1-DOF underactuated spring-linkage mechanism can adaptively follow a target path blocked by an obstacle via the deformations of spring elements [1, 2]. The simultaneous use of deformable spring elements and rigid links embodies the adaptability of an underactuated mechanism operating in a two-dimensional plane. The working principle of the underactuated spring-linkage mechanism is as follows; a 1-DOF underactuated spring-linkage mechanism can generate a specific path that minimizes the entire mechanism spring energy if no obstacle is present while it can go through significant elastic deformations to overcome an obstacle if there is any. The question is how to configure spring elements for a selected baseline rigid-link mechanism and determine their specific dimensions. Because one cannot pre-determine the number of spring elements to be used, it is inefficient and cumbersome to repeat many dimensional syntheses of spring elements by trying different numbers and configurations of spring elements. To be able to perform a streamlined synthesis of spring elements without many trials and errors, we propose a new optimization-based synthesis method, similar to the mechanism topology optimization [3, 4]. While earlier studies [3, 4] considered the synthesis of a rigid-link mechanism (without spring elements) only, our approach synthesizes spring configurations in an underactuated spring-linkage mechanism. In this respect, this work has newly performed the synthesis of spring configurations in underactuated spring-linkage mechanisms. The details of the proposed method, from formulation, analysis, to optimization, will be presented here. We will also show some numerical examples, such as the design of adaptive gait mechanisms and grippers, to demonstrate the validity and effectiveness of the proposed optimization-based synthesis method.

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Proportional topology optimisation with maximum entropy-based meshless method for minimum compliance and stress constrained problems

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Key Words: Maximum entropy meshless method, proportional topology optimisation, minimum compliance, stress constrained

In this paper proportional topology optimisation (PTO) with maximum entropy (maxent)-based meshless method is presented for two-dimensional linear elastic structures for both minimum compliance (PTOc) and stress constraint (PTOs) problems. The computation of maxent basis functions are efficient as compared to the standard moving least square (MLS) and possess a weak Kronecker delta properties leading to straightforward imposition of Dirichlet boundary conditions [1, 2, 3]. The PTO is a simple, non-gradient, accurate and efficient method compared to the standard topology optimisation methods [4]. A detailed and efficient implementation of the computational algorithms for both PTOc and PTOs are presented. The maxent basis functions are calculated only once at the start of simulation and used in each optimisation iteration. Young's modulus for each background cells is calculated using the modified solid isotropic material with penalisation (SIMP) method. A parametric study is also conducted on the degree of proportionality and history dependence of both PTOc and PTOs algorithms. A variety of numerical examples with simple and complex geometries, and structured and unstructured discretisations are presented to show the accuracy, efficiency and robustness of the developed computational algorithms. Both PTOc and PTOs algorithms can handle large topological changes and provide excellent optimisation convergence characteristics.

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Simultaneous Design of Rotating and Stationary Structural Parts of Fluid Flow Devices by Topology Optimization

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Key Words: Topology optimization, 2D swirl flow, Rotor-stator design, Discrete design variables, Integer linear programming

The fluid flow in rotating machinery is determined by the interaction between the working fluid, the rotating, and the stationary structural parts of the machines. Thus, the simultaneous design and optimization of rotating and stationary parts require modelling solid at different rotations. However, the standard fluid flow topology optimization method considers only a single stationary solid [1] or a single rotating solid [2]. Hence, this work presents a topology optimization formulation capable of optimizing structural parts at different rotations. Two mutually exclusive Darcy terms are added to the Navier-Stokes equations, with each Darcy term modelling a different rotation. The method employs two discrete design variable fields and considers three element phases: fluid, stator, and rotor. The fourth phase provided by the combination of the two discrete design variables is avoided by properly selecting the moving limits of the optimization algorithm. The optimization problem is solved by a TOBS-based approach [3]. The algorithm is applied to the design of radial and radial-axial machines. The fluid flow equations are solved by the Finite Element Method (FEM) and the sensitivity analysis follows the discrete adjoint approach.

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Structural Optimization Method Based on the Allen-Cahn Equation

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Key Words: *Allen-Cahn equation, Phase Field Method, Shape Optimization, Topology Optimization*

We introduce a new structural optimization method, which realize sequential topology and shape optimization, based on the Allen-Cahn equation with new expressions for double-well potential and source terms.
Takezawa et al. established a shape and topology optimization method with the phase-field method[1]. This method enables us to get an optimized shape which has clear boundary like the one obtained by the level-set method[2][3]. Also, this method doesn't require re-initialization, so the calculation is simply and easily achieved. On the other hand, it is well known that this method does not allow us to make a new hole during the optimization procedures. Here, we define two time-dependent evolutional equations; one is for the topology optimization, and the other is for the shape optimization. We firstly obtain an optimized configuration by the topology optimization, which allows us to generate holes, then we polish the first-step optimized configuration by the shape optimization. We verified the validity of our method through the several numerical examples.

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Topological Design of Thermal Conductors with Functionally Graded Composite Structure Using Machine Learning Based Material Properties

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Key Words: *Topology optimization, Thermal conduction, Functionally graded structure, Representative volume element, Machine learning*

This study presents a new design method for thermal conductors with functionally graded composite structures, which simultaneously optimizes the overall topological layout and the local fibrous material for high thermal conductivity. Periodic boundary conditions are imposed to unit structures configured with the design variables in the feasible set, and the corresponding anisotropic effective material properties of the composite unit microstructure can be obtained by the representative volume element (RVE) method. In addition, the machine learning method of neural network fitting is applied to discretized RVE data to build a design module to derive effective material properties according to the shape change of the unit structures [1]. In this study, with the objective function of minimizing the dissipation of heat transport potential capacity (or thermal compliance) and the multiple volume fraction constraints for each material type constituting the composite structure, thermal conduction optimization problems are formulated under various dimensions of the design domain and thermal boundary conditions. Numerical examples are introduced to verify the proposed method. Finally, the projection method is applied to the obtained topology optimization results, which converts the complex micro-scale structures to a manufacturable level [2].

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Topology optimization for mass minimization design of multi-material structures using *p*-norm function

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Key Words: *Level Set Method, Multi-Material Topology Optimization, P-norm Function*

Since the total mass of a multi-material structure is determined by the various composition ratios of each material, the mass minimization of the structure is basically a multi-objective optimization and, hence, it is not easy to obtain a single optimized solution. In particular, when multi-material topology optimization [1] that can derive a detailed distribution of each material within the design domain is performed, a designer can drive one meaningful optimized shape of the structure, however there can always be a better optimal solution with different material volume ratios. Although the multi-objective optimization methods are a great help in examining various design candidates of multi-material structures in this situation, they are still difficult to use, requiring a lot of parameter study and computation time for non-experienced engineers.

Thus, in this study, an efficient design method based on topology optimization that can easily examine various optimized shapes of multi-material structure for mass minimization. The optimization problem is formulated using a *p*-norm type objective function [2] that can give weighting factor to each material's mass rather than the actual mass of the structure. Since the ratio of each material to the total mass of the structure can be adjusted according to the value of the penalty factor of the *p*-norm function, it is possible to easily obtain various types of mass reduction designs that satisfy the target mechanical stiffness set as the design constraint and compare them with each other. Several 3D design examples were performed to confirm the usefulness of the proposed method and the effect of the penalty factor value on the optimized results. Since the composition ratio of each material consisting the entire structure can be controlled only by the value of the penalty factor and a consistent design direction can be confirmed, this study suggests an appropriate range of *p* values that designers can use.

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Topology optimization for maximizing fracture resistance using crack phase-field and reaction-diffusion-based level-set approach

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KEY WORDS: *Topology optimization, fracture resistance, phase filed model, reaction-diffusion equation*

Cracking is one of the most common failure modes and should be addressed since it could drastically decrease structural integrity and might lead to a serious incident. Therefore, enhancing the fracture toughness or structural persistence is of great importance in the engineering field. To maximize the fracture resistance of structures subjected to damage due to cracks, topology optimization considering crack propagation is one of the promising approaches.

Topology optimization for maximizing the fracture resistance of quasi-brittle composites is originally proposed by Xia et al [1] by combining the phase-field crack model and a gradient-based BESO optimization method and followed by Wu et al [2] who utilize a novel topological derivative in the level-set approach and adopted a reaction-diffusion equation to update the level-set function. We also explore the same objective with the latter approach but take the topological sensitivity to search for optimal topologies. Specifically, we derive the topological sensitivity to perform topology optimization for maximizing fracture resistance by combining the phase field fracture model and level-set approach with a reaction-diffusion equation. The effectiveness of the proposed updating process of the level-set function is investigated through several benchmark tests. In particular, the improvement of fracture resistance, number of design iterations, dependency of initial design are the objects of our interest.

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Topology Optimization of Binary Structures (TOBS) applied to stress-based problems considering geometry trimming

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Key Words: *Stress-based topology optimization, discrete variables, TOBS, geometry trimming*

Nowadays, stress-based topology optimization problems are well-known, but they are still a standing challenge. For continuum problems, there are three main issues to be overcome: the high nonlinearity relation between design variables and the stress values; the local nature of stress; and the singularity phenomenon. When considering discrete variables, the singularity problem is naturally avoided [1]. Thus, this work proposes a new approach to handle stress-based topology optimization problems by using the TOBS (Topology Optimization of Binary Structures) method [2] and geometry trimming (GT). The TOBS method is an optimization algorithm to update the design variables as binary values (0 or 1) by considering the linearization of the objective and constraint functions, and the subproblems created are solved using integer linear programming. GT is a technique to remove void regions of the domain so that the finite element analysis is performed only at the solid domain. Since TOBS gives clear 0-1 solution, the solid-void interfaces are easily identified. Then the jagged contours are smoothed, and a new domain is created. Because of the GT technique, re-meshing is necessary at each iteration. To avoid the discontinuity of the moving domain through the iterations, we propose to define two domains. The first one, called optimization domain, is fixed, and meshed only in the beginning of the optimization process. In the optimization domain the design variables are defined, and the mass constraint and its sensitivity are calculated. The second domain, called analysis domain, is the trimmed structure that needs to be re-meshed every iteration. It is where the finite element analysis, objective function, and its sensitivity are calculated. The TO procedure is performed in the optimization domain. Thus, the objective function sensitivity must be interpolated from the analysis domain to the optimization domain only where the design variables indicate solid regions. To avoid numerical instabilities, a spatial filtering technique is applied. The filter is also useful to extrapolate the objective sensitivities to void regions near the solid domain. This allows void elements to return to solid phase when necessary. This method is entirely implemented in Matlab and uses the LiveLink script of COMSOL only to generate the trimmed domain and mesh it. Numerical examples are presented to demonstrate the proposed method.

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Topology Optimization of Continuously Variable Stiffness Carbon Fiber Reinforced Plastic (CFRP) Structures with Level Set Method

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Key Words: *Topology Optimization, Fiber Path Design, CFRP Materials, Level Set Method*

The structural topology and fiber orientation play a very important role in the performance of carbon fiber reinforced plastic (CFRP) structures [1,2]. This study proposes a topology optimization approach for design of CFRP structures with continuously variable stiffness by using the level set method. The radial basis functions (RBFs) are employed to construct the level set function (LSF). In this way, the LSF can be formulated in a parameterized form. Fiber orientations are determined according to the LSF values at the nodes within elements [3]. The path of zero level set is extrapolated to other elements, and the fast marching method is employed as a re-initialization scheme in the optimization process to maintain the fiber paths.

In this study, two different design schemes are developed to conduct optimization of CFRP structures. One is the separate design scheme, in which conventional topology optimization with the level set method is first carried out with isotropic materials to determine clear structural boundaries. Then fiber path optimization can be performed based on the fixed topological boundaries defined by the RBF level set function. The second scheme is to carry out a parallel optimization of both structural topology and fiber paths, allowing to capture how fiber path affects structural topological boundaries.

Three illustrative examples are presented in this study to demonstrate the effectiveness of the proposed optimization method. Results indicate that optimized structures using the parallel optimization scheme offer better performances than the separate optimization scheme to a different extent, which implies that there may be considerable limits in the design space with the separate optimization scheme. The superiority of this study is that structural topology optimization and fiber path optimization are taken into account simultaneously. Besides, due to the inherent advantages of the level set method, when using advanced manufacturing techniques such as 3D printing, the fiber nozzle could move along the optimized fiber paths, and design of fiber nozzle route is no longer necessary compared with element-based fiber orientation design.

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Topology Optimization of Fluid-structure Interaction Problems with 2D Swirl Flow and Turbulence Models

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Key Words: Topology Optimization, Fluid-structure Interaction, 2D Swirl Flow, Turbulent Flow, TOBS Method, Integer Linear Programming

Design optimization of rotating structural parts, such as in turbomachinery, requires the solution of the Navier-Stokes equations that can include complex effects such as swirl flow, turbulence and fluid-solid equilibrium. While these physics have been employed successfully in the context of parametric and shape optimization, they represent considerable challenges for topology optimization. These challenges include the accurate modelling of fluid-solid walls, imposition of coupling conditions and convergence of the fluid-structure interaction (FSI) equations during optimization. This work employs a TOBS-based approach [1] that consistently produces well defined and smooth fluid-solid walls, an important step to add up extra physics or equations in the simulation during optimization. The structural compliance minimization problem subject to volume constraints is solved. The FSI problem is solved via the Finite Element Method considering axisymmetry. Rotational forces are imposed on the structural domain in the radial direction. The 2D swirl flow is governed by the Reynolds-Averaged Navier-Stokes (RANS) equations including a rotating wall in the shaft. The $k-\omega$ turbulence model is employed. Automatic differentiation is employed to compute the required sensitivities. A material model is included in the swirl flow terms to account for the sensitivities of the swirl flow loads on the structure. The optimization problem is solved by using Sequential Integer Linear Programming. Since solving a 3D-FSI topology optimization problem is computationally costly, the development of 2D swirl flow frameworks is of high interest. Results show that the proposed method can effectively achieve optimized designs of rotating structural parts under FSI loads.

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Topology Optimization of Multilayered Acoustic-Poroelastic-Elastic Structures for Sound Attenuation

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Key Words: Topology optimization, BESO, Multiphysics Problems, Poroelastic materials

Multilayered structures for sound attenuation have been explored in many scenarios, ranging from civil construction to automotive and aerospace industries. However, the proper multiphysics interactions comprised by acoustic-poroelastic-elastic structures are still challenging, especially when topology optimization techniques are involved. This work entails a new topology optimization methodology based on the Bi-directional Evolutionary Structural Optimization (BESO) approach to design bidimensional multilayered structures for sound absorption enhancements. The full modeling of poroelastic bodies is done by the mixed **u**/p technique, while the elastic and acoustic (air) materials are obtained by the degeneration of the latter, leading to the well-known elasto-dynamic and Helmholtz formulations, respectively. Such procedure is done in a systematic manner by the combination of the Finite Element Method (FEM) with the Unified Multi-Phase (UMP) modeling method, which in turn contributes to the development of material interpolation schemes suited for the application. In this scenario, the topology optimization problem is established as the maximization of the sound absorption coefficient, as composed by the summation of the time-averaged power dissipated through structural damping together with its corresponding viscous and thermal dissipative components. The numerical examples show the effectiveness of the proposed methodology, since it provides well-defined topologies with generally enhanced sound attenuation performances.

Topology optimization of rotational turbulent flow utilizing TOBS with geometry trimming method

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Key Words: *Topology Optimization, Swirl, Turbulent Flow, TOBS-GT*

Topology optimization (TO) of highly turbulent Flow is a challenge design problem specially when considering a rotational flow (swirl) around a shaft. This phenomenon has a wide range of applications in design of high-performance turbomachinery device such as compressors, mixers, turbines, and labyrinth seals. In the last decade, the improvement of fluidic device design has attracted significant attention and topology optimization is a feasible approach to achieve the best design for such a device. Here, we present a topology optimization method based on binary variables with geometry trimming (TOBS-GT) which considers the wall function to solve this problem. Thus, the method is implemented in COMSOL Multiphysics utilizing Reynolds Average Navier-Stokes (RANS) equation with k-ε and k-ω formulations for high Reynolds number considering a flow rotation around the shaft. The sensitivity analysis is calculated by using automatic differentiation. Topology optimization problem is solved using Integer Linear Programming (ILP). For each step, geometry trimming creates a CAD model with smooth wall for fluid region. Numerical examples from the literature are solved considering minimization of turbulent dissipation energy as objective function or in some cases maximization of turbulent dissipation energy and vorticity. Critical parameters such as Reynolds number at the inlet, shaft radius, objective function and rotation speed are investigated. The results indicate that rotation has a significant effect on the design of the fluidic device with rotational flow.

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Topology Optimization of structures reinforced with fiber considering stress constraint

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Key Words: Topology Optimization, Stress Constraint, Fiber Orientation

Several areas of Engineering, as aerospace and marine applications [1, 2], electronic industry [3], and civil engineering [4] are increasing the use of fiber-reinforced structures. In most cases, the main reason is their high strength-to-weight ratio and excellent fatigue resistance [5]. However, this is not the only reason. For the case of the concrete, the fiber-reinforced allows the creation of high-performance materials, and it is possible to project structures with non-conventional topologies using them. In the previous examples, the structures are composed of fiber and a material denominated matrix, where the reinforcement is placed. Besides, the structure's properties depend on how the fibers are oriented inside the matrix. For this reason, several works are proposed in the literature to determine the optimized fiber orientation. However, to consider the fiber orientation directly as a design variable can lead to a multiple local minima problem [6]. Particularly, there is one approach that avoids these problem considering candidate discrete angles to solve the optimization problem. This approach is implemented to solve linear and non-linear structural problems [6, 7, 8, 9, 10, 11]. Another approach is used to solve problems considering piezo composite materials, where sine and cosine function are approximated by Taylor series [12, 13]. However, a topic of research scarcely explored is the inclusion of stress constraint models in the topology optimization of composites materials [14]. In this work, the authors propose to solve the structural Topology Optimization problem considering local stress constraints for fiber-reinforced materials. The penalization for both material interpolation models is calculated automatically by including them as a design variable together with the pseudo-density. The grayscale issue is treated using the Guest projection with a proposed function to control the continuation on β variable. A benchmark example is solved to show the effectiveness of the method.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Topology optimization of subsonic compressible flow using the TOBS-GT method

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Key Words: Compressible flow, Subsonic, Topology optimization, TOBS-GT

Incompressible fluid flow includes a vast quantity of optimization engineering problems. However, depending on the flow characteristics, the compressibility of the fluid starts to be no longer negligible and the flow becomes compressible. Currently, the fields of energy generation and gas leakage control (where the flows are intrinsic compressible) have been receiving special attention in order to mitigate the greenhouse gases emissions and, consequently, climate change. To the best of the authors' knowledge, the work of [1] was the first to apply the topology optimization (TO) in laminar and compressible flows a density-based approach. Density-based models have been successfully applied to many fluid flow problems over the years. Nonetheless, the approach presents some well-known drawbacks. First, First, the optimization parameters have a high impact on the final result being often determined by a cumbersome trial and error process. Second, the presence of elements with intermediate pseudo-densities values, which may lead to artificial physics simulation. Recently, an alternative approach called Topology Optimization of Binary Structures with Geometry Trimming (TOBS-GT) was proposed by [2], aiming to reduce the influence of the optimization parameters and the appearance of gray regions. The TOBS-GT method consistently produces a clear interface between fluid and solid by trimming the solid regions from the design domain. This work expands the application of the TOBS-GT method to subsonic compressible flow problems under a low Reynolds regime. The objective function considered is the minimization of entropy generation. Three cases are evaluated, a traditional double pipe, a pipe bend, and a diffuser.

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Topology optimization of thermal fluid–structure systems

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Key Words: Level–set Method, Fluid Topology Optimization, Parallel Computing, Mesh Adaptation, FreeFEM-PETSc-Mmg

We propose a novel framework for the two- and three-dimensional topology optimization (TO) of a thermal fluid–structure system. The proposed design methodology uses a reaction-diffusion equation (RDE) for updating the level-set function based on the topological sensitivity. From the numerical point of view, two key ingredients are highlighted: (i) two different types of dynamic sparse grids (adaptive mesh) are used. More accurately speaking, body-fitted mesh allows the disjoint–reunion of a global mesh whose interfaces can be described by an implicitly defined surface (zero level-set). Anisotropic mesh adaptation is highly scalable with respect to the problem size, therefore can accelerate the overall computation; (ii) our framework uses FreeFEM for finite element analysis (FEA) and PETSc for distributed linear algebra. Efficient preconditioner techniques are utilized to solve the large-scale finite element systems. From an engineering standpoint, we construct a complete product development workflow including the preprocessing, TO, B-Rep conversion, and the numerical experiment. The performance of our methodology is demonstrated by solving a variety of optimization problems: mean compliance, minimal power dissipation, dry-/wet-fluid–structure interaction (FSI), natural convection, lift–drag, and fluid-to-fluid heat exchange. For comparison and for assessing our various techniques, we benchmark our designs against state-of-the-art works.

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Topology Optimization of Thin-Walled Structures with Body Conformal Adaptive Meshing

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Key Words: topology optimization, adaptive mesh, level-set method, length scale constraint

Thin-walled structures are widely seen in industrial systems. A computational synthesis to design such structures are demanded. This study proposes a high-precision topology optimization method for 3D thin-walled structures. Topology optimization generally uses a fixed mesh for the structural analysis model. Therefore, the interface representation between voids and materials is less accurate than surface-represented models due to staircase approximation or grayscale band of the interface. This accuracy issue may be acceptable if the designed structure is thick, i.e., the ratio of surface to volume is small. However, this discrepancy becomes nonnegligible when designing thin-walled structures due to the increased surface area to the volume. To overcome this issue, we incorporate an adaptive meshing scheme to eliminate the staircase approximation and grayscale band by meshing conforming to the solid/void interface.

The proposed method comprises a length scale constraint for uniform thickness and an adaptive meshing scheme. The uniform thickness is achieved by the minimum and maximum feature size constraints using Helmholtz partial differential equations[1]. For the adaptive meshing, we use MMG[2] for the implicit domain meshing, which can generate a conformal mesh separated by the level-set surface. By enhancing the binarization of the design variables on the conformal mesh, the performance analysis in the optimization process can be conducted accurately.

Numerical examples are provided to demonstrate the performance of the proposed method, including the accuracy improvement for the analysis compared to the conventional fixed meshes.

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Total Traction Equilibrium in Fluid-Structure Interactions with Porous Media

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Key Words: topology optimization, fluid-structure interactions, traction equilibrium

Fluid-structure interactions refer to problems where a deformable or a movable structure interacts with a flowing or a stationary fluid. A large body of research work has been dedicated to the numerical analysis of these interactions [1], and most multiphysics simulation packages - commercial and open source - include some degree of capability for solving these problems. However, the application of numerical design tools such as topology optimization to these problems is still lagging behind. This is mainly due to the multidisciplinary nature of the combined topology optimization of fluid-structure interactions problem and its strong nonlinear behavior resulting in numerous stability and convergence issues.

Since the first appearance of density-based topology optimization methods in the late 1980s, topology optimization has been extended to a huge range of single and multiphysics systems. In fluid flow, porous media is introduced along with some sort of penalization (typically Brinkman) to push the solution towards a 0/1 discrete state. The first appearance of high-fidelity *wet* topology optimization of fluid-structure interactions was in [2]. The fluid and solid computational domains overlapped such that the whole design domain - including the fluid-structure interface - could be optimized, hence the term *wet* topology optimization. In [2], the author extended the fluid-solid force coupling to the entire fluid domain including porous elements but only considered the hydrostatic component of the fluid stress tensor. The divergence theorem was utilized to transfer the integral from surface to volume. This step has a serious implication on the accuracy of the force coupling.

The novelty in this work can be summarized in two points: **(i)** we derived the traction equilibrium condition using the *total* stress tensor such that viscous forces are also considered, and **(ii)** we demonstrated the effect of the existence of sharp gradients in the fluid flow on the accuracy of the traction equilibrium condition.

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Arbitrary Negative Poisson's Ratio Metamaterial Microstructure Design by Topology Optimization Method

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Key Words: *Negative Poisson's ration, Metamaterial, Topology optimization, The further development of ABAQUS*

Since the concept of metamaterials was proposed in the early 21st century, after more than 20 years of development, it has gradually become an important branch of new material technology. With its excellent performance far exceeding natural materials and its designable and tunable characteristics, the arbitrary negative Poisson's ratio metamaterial has important research value and broad application prospects. In this paper, based on the topology optimization method, mechanical metamaterials of the arbitrary negative Poisson's ratio metamaterial are studied, and a novel programmable and tunable functional element design method with arbitrary negative Poisson's ratio metamaterials and structures is proposed. Its design idea combines optimization algorithms with human adjustments. When constructing a negative Poisson's ratio structural topology optimization model, directly constructing the objective function with the mathematical expression of negative Poisson's ratio will make the objective function highly nonlinear and make it difficult to analyze the sensitivity of the iterative process. Therefore, in this paper, the linear fitting method is used to construct a negative Poisson's ratio microstructure topology optimization objective function with linear characteristics. Based on the energy method and the homogenization method, a topology optimization that can quickly and accurately solve the negative Poisson's ratio is constructed. Based on the optimization model, a topological configuration and corresponding negative Poisson's ratio are obtained. Then, by introducing artificial design and using Python language, parametric modeling, GUI interface development, and calculation scripts for thermal stress homogenization methods for various element types were completed in turn on the ABAQUS platform. It not only realizes the function of quickly establishing a custom unit cell only by inputting a few parameters, but also deduces the unit cell structure under the specified Poisson's ratio, so as to realize the precise control of the Poisson's ratio of the unit cell, and truly realize the negative Programmability of Poisson's ratio metamaterial structures and tunable properties. The method in this paper not only avoids the highly nonlinear problem that occurs when the negative Poisson's ratio expression is used as the optimization function, but also reduces the complexity of the solution, providing a reference method for the design of negative Poisson's ratio microstructures.

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Considerations on the Updating Process in Density-based Topology Optimization Using the Modified Optimality Criteria Method

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Key Words: *Topology Optimization, Optimality Criteria Method, Density Method*

In recent years, design and production technologies have been growing rapidly in the automotive and electrical industries. Accordingly, numerical analysis has become very important. Numerical analysis requires various parameter settings. However, it should be noted that the results may vary depending on the parameter settings. The same can be said for the topology optimization, which is also attracting attention in the manufacturing industries. In this study, we focus on the update equation in the density-based topology optimization. In the topology optimizations based on the homogenization method and density method, the optimality criteria (OC) method[1] is employed as the update method. However, the conventional OC method requires the setting of several arbitrary parameters such as the move limit, which is a parameter to ensure stable updates, and weighting factor, which is a parameter for update speed. The results in Figures 1 to 3 are for the case when the move limit is not set and the penalization parameter is set to 6.0. When the modified OC method[2] is employed, the performance function does not increase as sharply as when the OC method is employed. Also, the weighting factor setting mentioned above is not necessary. In order to compare the OC method and modified OC method, the results for different parameter settings will also be presented.

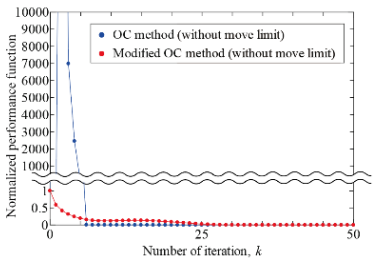

Fig. 1 History of normalized performance function.

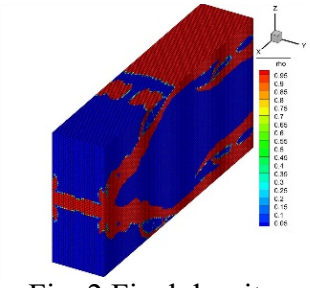

Fig. 2 Final density distribution when using the OC method.

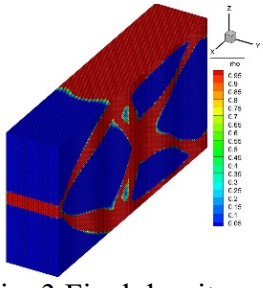

Fig. 3 Final density distribution when using the modified OC method.

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Design Optimization and Mechanical Property of Composite Materials with Embedded Cables

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Key Words: high integration; multifunction; composite materials; structural optimization

With the increasingly prominent contradiction between traditional aircraft and complex flight environment, the structure design has become more and more challenging. The integrating aircraft structure with different functional components such as flexible cables can improve the performance of the aircraft[1], which can make full use of the aircraft structure to quickly adapt to multiple missions in complex environment[2]. Integrated with different functional components, the multi-functional composite materials can have multiple functions such as support, protection, power distribution, data transmission and so on. At the same time, it can solve problems such as the difficult routing and the redundant size of cables in aircraft[3]. However, the embedded cables bring great challenges to the design and processing of composite materials. Structural design optimization of the carbon fiber composite material with embedded cables is realized in this paper by using co-simulation of ABAQUS and Python. Influence of component parameters on the mechanical properties of the composite material with embedded cables is further analyzed. According to the different load-bearing capacity in different areas of the composite material structure, topology optimization design under the constraint of embedded cables is considered, and the optimization of the layup angles of the composite material sub-area based on the multi-island genetic algorithm is further completed. The influence of the position of cables, the diameter of cables, and the distance between cables on the maximum bending stress of composite material structure is analyzed separately. Results of the research provide a certain theoretical basis for the design of composite materials with embedded cables, which can reduce the weight and cost of the aircraft structure.

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Flexoelectric Nanostructure Design using Explicit Topology Optimization

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Key Words: *Topology optimization, Flexoelectricity, Moving Morphable Void(MMV), Isogeometric analysis(IGA), Trimmed surface analysis(TSA)*

Flexoelectricity is the coupling between polarization and strain gradient. As the large strain gradient leads to a strong flexoelectric effect, the design of flexoelectric nano-structure via topology optimization has seen growing attentions. In the present work, an explicit topology optimization framework is proposed for flexoelectric structures design. To achieve this purpose, the Moving Morphable Void (MMV)-based approach is employed in the context of Isogeometric Analysis (IGA) combined with the Trimming Surface Analysis (TSA). Energy conversion factor and effective electric polarizability are respectively optimized to improve the flexoelectric performance of the nanostructure. Performing design under the explicit framework coupled with IGA can bring several advantages. Due to the use of NURBS basis functions of IGA, the required continuity in the approximation of the PDEs of flexoelectricity can be satisfied straightforwardly. Furthermore, with the use of the TSA technique, the occurrence of weak/grey material, which may cause numerical instability in flexoelectricity design, can be avoided. Also due to the explicit geometry description in MMV, the optimized result can be imported to the CAD system directly, which is significant for nanoscale structure from manufacturing perspective. Several representative numerical examples for topology optimization of flexoelectric structures are presented to demonstrate the effectiveness and advantages of the proposed approach.

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Topology and orientation optimization of fiber-reinforced composite structures considering fiber fabrication uncertainty

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Key Words: fiber-reinforced composites, orientation optimization, manufacturing uncertainty, robust topology optimization

In recent years, there has been increasing usage of fiber-reinforced composites in the aerospace and automobile due to their celebrated mechanical properties. So, huge research efforts are being made to develop methodologies for concurrent optimization of topology and fiber orientation of the structure. It is obvious that topology optimized continuous fiber-reinforced structures were impossible to manufacture other than additive manufacturing technology, often referred to be 3D printing. However, due to various environmental factors, there exists a gap between prescribed optimized fiber orientation and fiber orientation of manufactured composites. This presentation aims to present a robust topology optimization methodology of fiber-reinforced materials under fiber fabrication uncertainty. Our methodology is built upon SIMP type topology optimization, finite element analysis for numerical analysis and Method of Moving Asymptotes for updating design variables.

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Topology optmization for transient fluid-structure interaction

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Key Words: Topology optimization, Multiphysics Problems, transient system, fluid-structure interaction

This study proposes a topology optimization method for transient coupled fluid-structure interaction problems [1]. The transient FSI problem is formulated with the monolithic design approach combining the design variables and the governing equations. This developed approach allows a possibility to consider the effect of transient fluid-structure interaction on the topologically optimized layouts. Throughout the work, the analysis domain for fluid and structure is modelled with the unified monolithic approach at which the structure equation and the Navier-Stokes equation are coupled. With a fixed mesh and the design variables assigned to each finite element, the governing equations as well as the material properties are interpolated. This innovative modeling and analysis approaches provide accurate solutions to the strongly coupled governing equations. The adjoint approach for calculating the sensitivity information and a gradient-based optimizer are employed. Several numerical examples are solved to reveal the importance of the consideration of the transient fluid-structure interaction in structural optimization. In addition, these examples show that the present approach can control control of a transient FSI phenomena.

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Topology optimization of biodegradable composite structures with tunable time-changeable stiffness

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Key Words: *Topology optimization; Degradation modelling; Biodegradable metal matrix composite structures; time-changeable stiffness*

Recent advances in biomedical engineering have promoted the development of innovative metal implants that have integrated mechanical and biodegradable properties. Most of the existing implant designs were created by using a trial-and-error approach, which depends on the designer's experience. Alternatively, inverse design approaches, such as topology optimization, have evolved into an efficient design solution to optimize the structural and material layout within a given design domain. Here we introduce a novel multiscale topology optimization scheme to support the design of biodegradable metal matrix composite structures (BM-MCS) with tunable time-changeable stiffness. The effect of material degradation on the mechanical performance of the structure is considered by integrating a degradation simulation algorithm into the structural finite element (FE) analysis. The objective function is to minimize the structural compliance at macroscale in a certain number of time steps to realize sufficient structural integrity in the initial bone healing stage, and the different stiffness degeneration properties can be adjusted by changing the volume ratio of the two base constitutive biomaterials. The sensitivity of the above objective function concerning design variables was derived with considering the time-dependent degradation of the biomaterial. Several numerical design examples were presented and benchmarked with classical designs. Finally, several prototypes were fabricated by integrating additive manufacturing with casting technology. Collectively, this demonstrates the feasibility and effectiveness of the proposed inverse design method for additive manufacturing.

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Topology Optimization of Thermoelectric Devices with Mechanical Constraints

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Key Words: *Topology Optimization, Thermoelectric devices*

Thermoelectric devices have a wide range of application as energy converters due to their simplicity and reliability. Typical examples are energy recovery through heat-loss, solar energy, electronics cooling or temperature sensors [3]. The physics governing these devices is non-linear [2], making computational optimization demanding because of the many linear solves of large linear systems. However, during the last decade there have been several attempts to improve the performance of thermoelectric devices by changing their shape [1]. Furthermore, thermoelectric devices are subjected to thermal and installation related stresses that can reduce their efficiency [4].

The focus of this presentation is on the use of topology optimization and finite element methods to improve the performance of non-linear thermoelectrical devices and surrounding structures. By including the mechanical response of the device to external loads we can improve the thermoelectric device reliability with respect to installation loads and thermal cycling. It is also worth noting that these devices have an optimum operational point that will change with their geometry. For this reason, the operational point must also be optimized along with the topology of the device.

The procedure to follow for the optimization thermoelectric devices with 3D elements will be detailed together with different methods to improve computational performance and convergence. Finally, the results from the optimization for a single thermoelectric unit is showcased with the increased performance for different operational conditions.

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Inverse Design of Face-Like 3D Surfaces via Multi-material 4D Printing

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Key Words: *Inverse Design, 4D printing, Multimaterial, Shape Shifting, Machine Learning, Image Segmentation, Finite element analysis (FEA)*

Conventional methods for fabricating three-dimensional (3D) shell-like plastic objects include injection molding and direct 3D printing. However, injection molding requires expensive molds and machines, which is not suitable for high-mix, low-volume production. Direct 3D printing, on the other hand, is slow and consumes much sacrificial supporting material. In this paper, we develop an approach to overcoming those limitations by using multi-material four-dimensional (4D) printing. 4D printing integrates 3D printing and active material technologies to realize printed components transformed between different configurations upon heating [1-3]. Specifically, we aim to fabricate complicated 3D gridshells by transforming simple 2D grids by 4D printing. This is an inverse design problem in which one needs to determine the geometry and material configuration of a 2D grid given a target 3D gridshell. We print 2D grids consisting of rectangular arranged double-layered segments. Each layer is made of shape memory polymer (SMP55) or PLA, resulting in four combinations for each segment. The size and material combination of each 2D grid is specified to control both global and local curvatures of the deformed gridshell. As exemplars, we design three traditional Japanese “Noh masks” as the targets because Noh masks are an ideal model system as each mask has unique aesthetic features. Therefore, we conduct FEA for simulating the heating process and improving the design efficiency. Although FEA accelerates manual design, we build a machine learning model using image segmentation to predict 2D material patterns of corresponding 3D geometries. We show that the FEA simulations are consistent with the experimental results and successfully demonstrate the feasibility of our approach to producing complex 3D curved surfaces. Our method is eco-friendly, economical, and suitable for high-mix, low-volume production, and has considerable potential for further applications.

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Solid Mechanics within a Multi-Physics Modelling System for Analyzing Fusion Reactor Blanket Designs

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Key Words: *Coupled solvers, fusion reactors, digital twin*

Fusion energy systems require highly complex multi-physics models for understanding and optimizing performance. This is especially true for the blanket, the device where heat is extracted for power generation as well as tritium created from transmuted lithium, necessary for fuel production. In their most typical form, a fusion blanket requires coupling physical processes including radiation transport with isotope transmutation and depletion, thermo-hydraulics, quasi-static electromagnetics, solid mechanics, and heat transfer. More radical designs may include high-temperature gas flows and/or liquid metal free-surface flows facilitated by surface tension. Coupling between different physical processes may occur through the volume (radiation-induced heating and damage, Lorentz forces, Joule heating) and through coupling via surfaces (fluid-structure interaction, conjugate heat transfer). The Fusion Energy Reactor Models Integrator (FERMI) code suite is envisioned as a tool to enable these complex analyses, both to de-risk designs as well as provide a means towards optimization thereof. A range of solvers will be coupled in a single multiphysics simulation environment using the open-source coupling library preCICE. A selection of different electro-thermal-hydraulics and neutronics solvers will be coupled together along with the structural mechanics package Diablo for simulation of a blanket design. We analyze the performance and suitability of various coupling strategies in the context of the analysis of a conceptual blanket design.

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3D Topology Optimization of an Axisymmetric Wheel and Axle Structure with Orthotropic Constitutive Properties

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Key Words: *Topology Optimization, Design Automation, Machine Synthesis, Variable Loading*

In this work, we present a topology optimization methodology for automatically designing axisymmetric structures with arbitrary boundary conditions, arbitrarily shaped finite element meshes and design domains, and variable loads. We use the design problem of a wheelset: a rolling structure where wheels are fixed to the ends of an axle. Believed to be the first invention of the wheel used for transporting cargo out of early mines in the Carpathian Mountains [1], these wheelsets could conceivably have been crafted from wooden logs available near the mine entrances. To reduce the amount of work required to push heavy mine cars, the axles would have been made as thin as possible to minimize rolling resistance caused by friction at the surface of the axle. We replicate this historical design process using our modern and automated topology optimization algorithm.

To achieve an axisymmetric geometry while retaining the ability to apply arbitrary load and support boundary conditions, we use a manufacturing constraint in the form of a milling filter [2] that we have modified and extended as a 3D turning filter. The filter enforces axisymmetry of the density design variables about the symmetry axis, and in our implementation, we discretize rectangular shaped design domains using structured grids of finite elements. This produces geometries that can be manufactured by cutting a block of material using a turning machine tool such as a lathe. For modelling the axisymmetric material properties of a wooden log, we use orthotropic constitutive properties in a cylindrical coordinate system of longitudinal, radial, and tangential directions. Each element in the mesh is assigned stiffness properties corresponding to the constitutive matrix rotated according to the local orientation of the element. The stiffness of intermediate density material is then interpolated and penalized using the SIMP (Solid Isotropic Material with Penalization) method applied to the orthotropic constitutive matrix, or SOMP (Solid Orthotropic Material with Penalization).

The optimization problem is set up such that a wheelset structure is automatically generated given the simple objective of minimizing the radius of the axle and the mass of the structure, subject to a structural compliance constraint. The load is applied to the surface of the axle, whose geometry changes during the optimization process. This makes the wheelset structure a design-dependent loading problem; however, we do not apply any restrictions on the location of the load. Instead, we allow the numerical optimization process to find the optimal location along the axle's surface by treating the load coordinates as design variables [3]. We ensure that the load remains applied to the solid-void interface by projecting a moveable void space radially outward from the load application area. Ultimately, our proposed methodology successfully synthesizes a primitive wheelset geometry depicting circular discs connected to the ends of a narrow cylindrical axle.

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15th World Congress on Computational Mechanics (WCCM-XV)
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A Geometric Feature-Mapping Approach to Buckling and Fail-Safety Criteria in Topology Optimization

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Key Words: Topology Optimization, Geometry Projection, Stability, Redundancy

Stability and redundancy requirements can be critical to structures in many applications. In civil and aerospace contexts, unstable or damage-intolerant designs can render catastrophic consequences. Despite the clear importance of stability and redundancy, the thin and fully-stressed members typical of stiffness or strength optimized designs are diametrically opposed to these requirements.

Stability and buckling have endowed considerable attention since the onset of structural optimization. In truss optimization, local stability has been imposed via stress or displacement constraints on individual members. However, only a small number of works consider buckling in topology optimization of continua. In this setting, nearly all works consider a linearized bifurcation-buckling analysis. However, a geometric feature-mapping topology optimization approach provides direct representation and control of distinct structural members in a continuum setting. This enables certain local buckling modes to be intuitively and efficiently stabilized via geometric criteria in a continuum topology optimization.

Redundancy is essential to the safety of structures in the case of damage. If all structural members are indispensable, then only a small amount of damage can result in complete structural failure. In truss topology optimization, damage to the structure is modeled by eliminating or eroding a truss element. However, in continuum topology optimization, it is not straightforward to remove a distinct structural member. Damage scenarios in a continuum setting are often considered by removing patches of a fixed size, shape and location, or by degrading the entire structure by offsetting the boundary. A feature-mapping approach can enable modeling damage to the structure consistently with established fail-safe design principles by removing distinct geometric members from the design.

In this work, we exploit the underlying geometric design representation of the geometry projection method to formulate optimization constraints that heuristically increase buckling load factor and promote structural redundancy. This approach addresses buckling and fail-safety design requirements at a substantially lower computational cost than a purely physics-based approach. We demonstrate the efficacy and efficiency of our method via numerical examples.

Case Number: AFRL-2021-4446

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A Practicable Two-material Interpolation Method for Isotropic Brittle-ductile Topology Optimization

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Key Words: *Topology Optimization, Nonlinear Composite Structures*

The purpose of this study is to develop an optimal design method for improving both strength and toughness for composite structures that combine brittle and ductile materials. Based on the basic topology optimization method using SIMP, we propose one idea about the material representation method in a simple and easy-to-control scheme: interpolation of nonlinear material constitutive law.

The well-known composite structure of reinforced concrete has both high strength and toughness in the entire structure by supplementing concrete with high compressive strength but is fragile to tensile strength with reinforcing bars that can be tenaciously deformed. In this way, by combining two types of materials with different properties, it is possible to realize ideal mechanical behavior as a structure that is "brittle-ductile" There is still room for further investigation in the geometric design of such composite structures, and there seems to be an opportunity to improve performance by optimization simulation.

In the topology optimization method based on SIMP, a few material parameters such as Young's modulus are interpolated in order to express the mechanical behavior of a phase in which a solid material and a void or two different materials are mixed. However, when the concept is applied to a complex nonlinear material that switches discontinuously at a threshold with a stress-strain relationship or exhibits softening behavior, the evaluation function and the optimization problem become non-convex or discontinuous. When such an irrational problem occurs, the design variables vibrate and stay in grayscale, making it extremely difficult to reach the optimum solution by the optimization algorithm. Therefore, usually, the instability is mitigated to a level where the calculation can be executed by finely tuning the interior parameters and filtering settings, but in that case, the calculation result strongly depends on these settings, and the degree of freedom in design is not a little lost.

In this study, we assume a two-phase material consisting of a unilateral damage material and a von Mises elastoplastic material, and interpolate the material parameters between these materials. Therefore, we limit the target of interpolation to material parameters such as Young's modulus, initial yield stress, and initial damage strain, and try to formulate as simple as possible. This maximizes the effort and impact of tuning to mitigate optimization instability and improves the ease of handling the simulation. In this presentation, we will show some optimization results assuming a steel-concrete composite and discuss the mechanical rationality, numerical stability, and dependence of the optimal solution on interior parameters.

An Evolutionary Approach to Stress-constrained Topology Optimization

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Key Words: *Topology Optimization, BESO, Strength Design, Industrial Application*

We proposed recently an evolutionary approach to stress-constrained topology optimization using Bi-directional Evolutionary Structural Optimization (BESO) method. The discrete nature of the BESO avoids naturally the well-known "singularity" problem in density-based methods due to the degenerated materials. The p-norm stress aggregation scheme is adopted for the measure of global stress level. The compliance objective is augmented with the aggregated stress constraints by introducing one or multiple Lagrange multipliers. The Lagrange multipliers are employed to yield compromised designs between compliance and stresses. A computationally efficient sensitivity number formulation is derived from the adjoint sensitivity of the global stress measure. With regard to the highly nonlinear stress behaviour, both sensitivity numbers and topology variables are filtered to stabilize the optimization procedure; meanwhile, the filtered sensitivity numbers are further stabilized with their historical information. The method has been shown efficient, practical and easy-to-implement through a series of benchmark designs including the L-bracket benchmark. A series of comparison study has been conducted to test the feasibility of the method on the L-bracket benchmark design problem. The method has also been applied for the design of a typical aircraft engine bracket considering multiple practical load conditions. The resulting bracket topology from stress-constrained design is further smoothed and detailed using basic CAD (Computer-Aided Design) primitives. Numerical results show that the reconstructed bracket design evidently outperforms than the original bracket design in terms of weight, stiffness and strength.

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Comparative Study of Topology Optimization of Thermoelastic Structures considering Finite Strain Condition

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Key Words: *Topology optimization, Thermoelastic compliance, Structural nonlinearity*

In the topology optimization of a structure experiencing both thermal and mechanical loads (i.e., thermoelastic loads), consideration of the structural nonlinearity is crucial because the optimality of the resulting design is highly deteriorated otherwise. However, the choice of the objective function of thermoelastic compliances, which is widely used to maximize the stiffness of the structure, is limited in the finite strain setting because the thermoelastic load cannot be linearly decomposed into the mechanical and thermal ones. For example, the mean compliance function that is an inner product of total displacement and the sum of the thermal and mechanical load is not available yet the function is one of the most widely used objective function due to its resemblance to the strain energy. In this respect, the end compliance and strain energy functions are used as the alternative to the mean compliance. However, their respective results, including the optimized layouts, have not been discussed. Therefore, this study examines the differences between two notable thermoelastic compliances in topology optimization considering structural nonlinearity: end compliance and strain energy.
This talk addresses two main findings in the study. First, we carefully examine the optimized layouts that depend on the objective functions and thermoelastic loading conditions. Through the examination, we revealed the optimality of the layout through the re-analysis, and at the same time, the changes of design capability leveraging the fact that the one can have negative value while the other is not. Lastly, the same objective functions are optimized in the structurally linear case and compared with the nonlinear ones, again emphasizing the importance of finite strain formulation in thermoelastic topology optimization.

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Concurrent Topology Optimization of Parts and Supports for Additive Manufacturing Considering Thermal Deformation

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Key Words: *Topology optimization, Additive Manufacturing, AM-process simulation, thermal deformation, inherent strain method.*

In metal additive manufacturing (AM) e.g. selective laser melting, thermal deformation is an important factor affecting the manufacturing quality, improper control of which will jeopardize the size accuracy of the final prototype and even lead to manufacturing failure caused by the crash between the printed part and the powder re-coater. This work presents a density based topology optimization approach to concurrently design parts and supports for a perfect match between mechanical properties and manufacturing qualities. A layer-by-layer AM process simulation model based on an inherent strain method is developed to capture the thermal deformation during the AM process, which is further developed into a novel thermal deformation constraint and incorporated into the topology optimization model. Besides, an overhang constraint and a two-field based length scale control formulation are also considered, ensuring the overall manufacturability. With the proposed approach, lightweight structures with optimized mechanical properties and controlled thermal deformation can be obtained. Numerical examples are given to demonstrate the applicability of the proposed approach.

Concurrent Topology Optimization of Two-Scale Transient Heat Analysis Considering Size Effect

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Key Words: *Concurrent topology optimization, Multi-scale, Transient heat, Size effect*

Nowadays, topology optimization and additive manufacturing are widely used to design and fabricate heat dissipation structures [1], and many innovative designs are proposed due to their superb capabilities, e.g., free-form design, printing custom shapes, and rapid fabrication. For heat dissipation problems, lattice and porous structures with a high surface area frequently appear as the optimal layout. To design this kind of structure, multi-scale topology optimization which includes characteristics of heat dissipation of lattice and porous structures is required to be adopted. However, only a few studies have investigated topology optimization by not only taking into account the multi-scale heat behaviour but also transient heat analysis.

In the present study, a concurrent two-scale topology optimization framework for transient heat analysis is proposed. The homogenization method which is capable of considering the size effect of microscopic heat transfer is adopted [2] to deal with the multi-scale analysis of lattice and porous structures. Heat compliance is chosen to be an objective function, and then analytical sensitivity formulations are derived for each scale by using the adjoint variable method. Selected numerical examples are used to demonstrate the robust performance of the proposed framework. The analysis shows that the framework captures not only the transient heat but also the size effect of the microstructure in a transient heat analysis.

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Deformation Clustering Methods for Topologically Optimized Structures under Crash Load based on Displacement Time Series

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Key Words: *Deformation Behavior, Topology Optimization, Crash Load, Clustering, Time Series data, Dynamic Time Warping*

Multi-objective topology optimization has been receiving more and more attention in structural design recently. It attempts to maximize several performance objectives by redistributing the material in a design space for a given set of boundary conditions and constraints, yielding many Pareto-optimal solutions. However, the high number of solutions makes it difficult to identify preferred designs. Therefore, an automated way of summarizing solutions is needed for selecting interesting designs according to certain criteria, such as crashworthiness, deformation, and stress state. One approach for summarization is to cluster similar designs and obtain design representatives based on a suitable metric [1]. For example, with Euclidean distance of the objective vectors as the metric, design groups with similar performance can be identified and only the representative designs from different clusters may be analyzed. However, previous research has not dealt with deformation-related time-series data and structures with different topology. Since the non-linear dynamic behavior of designs is important in various fields such as vehicular crashworthiness, clustering methods based on the time-dependent behavior of structures is proposed here using metrics of time-series, such as DTW (Dynamic Time Warping) [2], for the comparison of displacement data of selected points on the structure. This is combined with clustering techniques such as *k*-Medoids [3] and OPTICS (Ordering Points To Identify the Clustering Structure) [4], and we investigate the use of unsupervised learning methods to identify and group similar designs using the time series of nodal displacement data. In the first part, we create artificial time-series datasets using mass-spring systems and a beam structure to validate the proposed methods. Each dataset has clusters of data with distinct behavior such as different periods or modes. Then, we find that the combination of DTW and OPTICS can identify the clusters of similar behavior accurately. In the second part, we apply these methods to a more realistic, engineering dataset which contains the crash behavior of topologically-optimized designs. We identify similar structures and obtain representative designs from each cluster, demonstrating the capability of our method for analyzing dynamic behavior, which supports the designers in selecting representative structures based on deformation data at the early stages of design process.

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Density-based Multi-material Topology Optimization Method Considering Strengths of Both Solids and the Interface

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Key Words: *Topology optimization, Multi-material, Interface representation, Stress constraint*

In recent years, the use of multi-material has been paid attention in the field of structural design to reduce weight and increase stiffness and strength. In order to make the most of the advantages of this multi-material technology, design techniques that effectively utilize materials with different properties in the right places are required. Therefore, a series of studies on the multi-material topology optimization has been actively pursued.

However, studies on multi-material topology optimization have been limited to extending single-material models, such as the SIMP method and level-set method, to multiphase materials. On the other hand, few studies take into account the strength of each material. Furthermore, the interfacial strengths of different materials are rarely considered, which often causes damage in structure.

One of the reasons for this is the difficulty in representing the bonding behavior. In density-based methods, such as the SIMP method, it is difficult to explicitly reproduce the interface and its bonding effect although it is easy to handle. On the contrary, the level-set method could represent the interface explicitly, the optimization results may be highly dependent on the initial configuration of the interface. In a recent paper, a level set method that takes into account the strength of the material interface was proposed by Liu et al[1].

In this study, we will develop a topology optimization method considering strength of each solid material and the interface simultaneously. We extend the graded interface proposed by Clausen et al[2] and Chu et al[3] to represent the interfacial strength. By comparing the optimal layout obtained by the proposed method with the ones obtained by the conventional mean compliance minimization problem, it is shown that the proposed method is more suitable for the actual design.

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Length Scale Control Schemes for Bi-directional Evolutionary Structural Optimization Method and its Application to Shell-infill Structures

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Key Words: *Topology optimization, BESO, P-norm, Skeleton, Length scale control, Infill architecture*

This research develops length scale control schemes for Bi-directional Evolutionary Structural Optimization (BESO) method, enabling an enhanced and flexible control of the method on structural member sizes. Specifically, the maximum length scale control is achieved by constraining local material volumes below a threshold value, which is determined upon the allowed maximum length. The massive per-element volume constraints are aggregated by the p-norm global measure. The aggregated volume constraint is augmented to the conventional compliance design objective through a Lagrange multiplier. On the other hand, the minimum length scale control is achieved by a post-processing modification of local feature according to the skeleton detected from a preliminarily optimized topology. The sensitivity numbers of the local structural features that violate the minimum length scale constraint are compensated during the post-processing modification. The effective and efficient of the proposed schemes in controlling both the maximum and minimum structural length scales are demonstrated by 2D and 3D benchmark design. Meanwhile, the proposed method accounting for length scale control can efficiently generate porous lattice structures, making it a powerful means for the infill architecture design. And it is successfully applied to the infill architecture design of shell-infill structures. Both numerical and experimental results show that the achieved shell-infill MBB beams outperform than the reference design with uniform lattice infill of the same weight in terms of stiffness and fracture resistance.

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Microstructure Control through Topology Optimization for Additive Manufacturing

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Key Words: Thermal history, Microstructure, Wire and Arc Additive Manufacturing (WAAM), Topology Optimization

In Wire and Arc Additive Manufacturing (WAAM), a metal wire is melted and deposited simultaneously along a predefined deposition path using a robotic arm. WAAM is used to manufacture large-scale structures such as ship propellers and airplane components. Mechanical behaviour of a WAAM part depends, among others, on microstructure development during the manufacturing process. Evolution of microstructure is dictated by the thermal history experienced by the part. For high strength low alloy steels, time spent by a material point between a critical temperature range $800°C - 500°C$ ($t_{8/5}$) affects the local microstructure development and, consequently, yield strength [1, 2]. As the thermal history of a material point during WAAM is influenced by the part geometry, this offers an opportunity to tailor mechanical properties through design.

In this study, we present a new method to control $t_{8/5}$ of critical structural regions through topology optimization. Firstly, the thermal history experienced by critical structural regions is evaluated through a simplified process modelling. In the process model, to simulate material deposition in WAAM, finite element activation approach is used. The finite elements are activated in layer-by-layer manner. For a particular layer, elements associated to it and previous layers are activated. A heat flux is subjected to the top surface of the finite elements associated to the latest activated layer for a particular period of time to simulate the heat input in WAAM. Secondly, it is essential to evaluate design sensitivities of $t_{8/5}$ for topology optimization, therefore, a continuous and differentiable approach is proposed to evaluate $t_{8/5}$ of critical structural regions. Thereafter, a study will be shown in which the effect of design changes on $t_{8/5}$ is investigated. The results show that overhanging features orthogonal to the deposition directions of layers have high $t_{8/5}$. High $t_{8/5}$ can lead to low yield strength due to development of microstructure with high volume fractions of solid phases with low hardness [1]. Thus, in this work we present a novel integrated approach to generate optimized structural design considering the stress generated in the critical regions and yield strength which is result of the microstructure development during the manufacturing process.

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Microstructure Optimization for One-Dimensional Nonlinear Constitutive Laws Under Tensile Loading

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Key Words: Topology Optimization, Microstructure Tailoring, Nonlinear Optimization, Finite Strain Optimization, Constitutive Laws

Topology optimization has previously been used to tailor microstructural motifs towards the realization of specific desired bulk material properties. However, optimizing a nonlinear microstructure geometry has received limited attention. Most efforts toward matching a nonlinear constitutive law have either focused on one-dimensional bar and beam problems [1], or, within continuum designs, on the simpler problem of minimizing or maximizing mechanical response at single loading conditions of interest, rather than matching responses of a single designed structure throughout a range of loading conditions.

We explore microstructure optimization to induce softening and stiffening in nonlinear stress-strain behavior in a two-dimensional (2D) continuum setting. We employ a geometrically nonlinear, finite strain, displacement control level set topology optimization scheme. The use of the level set method allows us to avoid the intermediate density elements typically encountered in density-based optimization. Within the context of a 2D continuum, we demonstrate nonlinear constitutive law matching across a range of displacements, within the vicinity of a local optimum. We further explore the use of various guiding metrics, including strain energy measures and polynomial fitting, in order to expand the capabilities of this method to target desired stress-strain curves across a broader range of the highly nonlinear design space, so that a wide range of desired constitutive laws can be achieved.

The ongoing maturation of this method aims to physically realize systems that have previously only been theorized and simulated, which require the expression of specific nonlinear stress-strain curves not easily found in existing materials or designs [2]. The ability to optimize for any desired general constitutive law shape will enable exciting research opportunities in metamaterials, nonlinear dynamics, waves, and impact absorption applications.

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Multi-material Topology Optimization Model using the Multi-phase-field Method

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Key Words: *Topology Optimization, Multi-material, Multi-phase-field Method*

Topology optimization is the most flexible method in structural design, and its practicality is increasing because the development of additive manufacturing (AM) has facilitated the creation of products with complex shapes. In addition, AM has recently enabled the fabrication of products using multiple materials. Therefore, an optimization technique that includes the degree of freedom of both shapes and materials should be established.

The solid isotropic material with penalization method, which is widely used for the topology optimization of a single material, is difficult to be feasibly extended to multiple materials. The phase-field method is a stable interface tracking method, which has been applied for topology optimization of multiple materials [1, 2]; however, a definitive method has not yet been developed. In this study, we apply the multi-phase-field model—which has been used for multiphase and polycrystalline problems in materials science—for the topology optimization of multiple materials.

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On geometrically Nonlinear Stability Constraints in Topology Optimization

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Key Words: *Topology optimization, nonlinear geometry, stability constraints.*

Stability constraints play an important role in structural optimization problems to ensure that optimized designs can safely support the intended loads without undergoing large displacements, or even collapse, due to instabilities such as buckling. Topology optimization problems that minimize linear compliance (maximize linear stiffness) often result in structures with thin members under compression that are susceptible to failure by buckling instability. This is a well-known issue and has led to research on including stability constraints in topology optimization problems. This is usually achieved by estimating the critical load factor by a linear buckling analysis [1,2]. However, buckling is inherently a geometrically nonlinear problem and the linear approximation may over or underestimate the true load capacity of the structure.

Therefore, a geometrically nonlinear analysis can be used to compute the critical load factor more accurately [3]. However, this approach has received less attention, possibly because of the high computational cost of the nonlinear analysis. Another issue is that accurately identifying the limit point for the critical load level is difficult because the tangent stiffness matrix becomes singular at a limit point. Thus, in practice, we can only obtain a solution near a limit point [3]. This leads to inaccuracies in the computed gradients, which can cause convergence issues when using gradient-based optimizers, especially if the geometrically nonlinear stability constraint is difficult to satisfy (i.e. the optimal design with a stability constraint is significantly different to one without).

Two strategies are proposed to overcome this issue, which are tested using benchmark problems. The first strategy is simply to "go slow" by using small updates of the design variables each iteration, which reduces the influence of inaccurate gradients on convergence. This strategy leads to more stable convergence, but extra computational cost, as more design iterations are required. However, computational cost may be reduced by reusing information from the previous iteration to speed up convergence of the geometrically nonlinear analysis. The second strategy is to achieve the desired stability constraint using an implicit formulation based on nonlinear stiffness measures. This strategy reduces computational cost and avoids issues of inaccurate gradients, as the limit point is not explicitly computed. However, because stability is only implicitly enforced, this strategy may result in an overdesigned structure.

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Optimal Design for Continuous Fiber Layout of 3D-printing FRP

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Key Words: *Additive Manufacturing, 3D-printer, Fiber Reinforced Polymer, Optimization*

In the last few decades, additive manufacturing technology has been actively developed and various materials such as metal, resin, ceramic, cement and eventually continuous fiber reinforced polymer (FRP) can be printed by 3D-printer. The emergence of 3D-printing technology for continuous FRP is expected to open up a new era of manufacturing in various engineering fields. The most important feature of this new technology is the ability to freely change the arrangement and orientation of continuous fibers in the laminate plane, which have superior strength and stiffness to short fibers. However, the design method of continuous reinforced fiber orientation of FRP which is premised to be produced by 3D-printer, has yet to be deeply investigated. Under this circumstance, this study aims to establish an optimal design method for 3DP-FRP.

A conventional design method for 3DP-FRP is a density-based approach based on the SIMP [1] in consideration with anisotropy. In this method, each discretized element based on the finite element method has two design variables, material density (fiber arrangement) and angle (fiber orientation), and then the objective function is minimized/maximized by updating these variables [2]. Since the fibers are discretized, the continuity of fibers, which is the main feature of 3DP-FRP, cannot be expressed in this framework. As a result, it is necessary to introduce a filter to ensure the continuity of the fibers, or a post-process procedure to joint them together: this kind of post process may lose the mechanical reliability to the optimal layout.

To avoid such a problem, we propose a method in which the design variables are defined at the nodes of finite elements. The isosurfaces created by these values are regarded as fiber paths, and the arrangement and orientation of the continuous fibers are optimized by varying the nodal values instead of the density and angle.

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Preliminary Study on Multi-material Dynamic Topology Optimization based on Generalized Maxwell Model

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Key Words: *Topology Optimization, Dynamic Structural Problem, Viscoelasticity, Generalized Maxwell Model*

In dynamic structural systems, the capability to restore or dissipate energy is one of the priorities when concerning the optimal dynamic performance design [1]. To achieve this purpose, viscoelastic material such as rubber-like material is often applied. However, the concern of how to represent the characteristics of real dynamic response has yet to be clarified [2], [3]. To fulfil this design, development of multi-material topology optimization considering dynamic loading with a realistic viscoelastic material model is required.
In the present study, we addresses a design scheme for maximization of storage and/or loss energy under dynamic loading assuming viscoelastic bi-material. The generalized Maxwell model, which shows good consistency with viscoelastic performance, is used with the SIMP-like interpolation scheme. For the sensitivity analysis, an analytical adjoint variables method is used.
Finally, the proposed method is verified by a series of numerical examples.

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Structure Topology Optimization of Asymmetric Material with Prescribed Eigenfrequency Band

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Key Words: *Structure topology optimization, Granular material model, Tension-compression asymmetry material, Eigenfrequency optimization, Interval frequency topology optimization*

Granular material is an aggregate formed by numerous discrete solid particles through particle-to-particle interactions. It is ubiquitous in nature, daily life and engineering applications. Due to the tension-compression asymmetry of granular materials under external loadings, this fields becomes a hot field in bionics techniques and simulating the mechanic behaviours of bio-structure. This paper uses the method of micro mechanics, which bridges the micro-scale structure and the macro-scale mechanical phenomena. The macroscopic constitutive equation of granular material is established by the stiffness coefficient between particles. Topological optimization of structures composed of granular materials can create unique structures. When the external exciting frequency is approximating to some order of eigenfrequency in structure, the system will resonate. To avoid resonance of structure resulted from external exciting source, this work proposed the mathematical formulation to adjust eigenfrequency band between two consecutive eigenfrequencies of the granular material structure. The mathematical formulation of topology optimization can be stated as follows, in which difference of successive two frequencies for the structure was taken as objective and constitutive equation of cementitious was applied.

Benchmark problems are optimized to verify the correctness and effectiveness of the proposed mathematical formulation. The effect of granular material structure on the structural topology was investigated. Resultant topologies show that the dynamic topology optimized design obtained from the newly proposed material model is different from the traditional material design due to the tension-compression asymmetry at the microscopic scale. Additionally, the damage to the structure caused by resonance is effectively avoided through topology optimization.

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Thermostructural Topology Optimization of a Heat Exchanger with Stress Constraints

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Key Words: *Topology Optimization, Heat Exchanger Design, Geometric Projection, Design-Dependent Convection Loads, Coupled Thermoelastic Analysis, Adjoint Sensitivity Analysis*

The application of topology optimization to the design of heat exchangers has not been explored in detail. Therefore, we present a method for designing heat exchangers with geometric projection and density-based topology optimization. The goal of the optimization process is to minimize the maximum von Mises stress caused by thermal expansion within the heat exchanger, subject to a constraint on thermal efficiency. The locations and sizes of the air channels are the design variables used to parameterize the Heat Exchanger geometry, and those air channels are projected onto the design domain via geometric projection [1]. Iga's method for formulating design-dependent heat convection loads [2] is modified to model heat transfer along the projected air channel boundaries. A smooth Hat function is used to identify the elements along the material interface which forms the boundaries of the air channels through which heat convection occurs. A coupled thermoelastic model is developed using finite element analysis, and the design sensitivities are derived and evaluated using an adjoint analytical method. The interpolation of both the thermal and elastic material properties is based on the standard Solid Isotropic Material with Penalization (SIMP) method. Results are presented for a varying range of temperature difference between the inner and outer fluid streams. Results show that the maximum local stress within the optimized heat exchanger can be decreased significantly to avoid exceeding the yield strength of the material. Future work will include extending this framework to three dimensions where the number of plate layers and faces can also be modified during the optimization process. In addition, the optimization process will be developed further to maximize the transfer of heat from the hot fluid within the air channels to the surrounding cooler fluid.

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Topology Optimization for Unsteady State Thermal-Fluid Problems

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Key Words: *Topology optimization, thermal design, Multi-physics*

Topology optimization is attracting attention as a powerful design tool that can determine the optimum structural layout and material arrangement, and has been introduced in various engineering fields. In addition, topology optimization technology will be required more and more in the future because it has a high affinity with a next-generation manufacturing, namely additive manufacturing.

Thermal design, which is particularly important for electronic devices, is one of the representative engineering problems in which many beneficial results have reported with topology optimization [1], [2]. However, only a few studies have taken unsteady state thermal-fluid problem into consideration. In actual design problems, there are lots of cases in which temporal changes in temperature distribution are important rather than steady state.

In this study, the framework of a density-based topology optimization method for unsteady thermal-fluid problem is proposed. The governing equations are unsteady-state imcompressible Naiver-Stokes equation and thermal convection-diffusion equation, discretized with stabilized finite element method. The design sensitivity is computed accurately based on the adjoint variable method. The numerical analysis shows that the proposed framework captures the transient effect correctly and the results of optimization are physically reliable.

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Topology Optimization Incorporating the Adjoint Lattice Boltzmann Method for Steady and Unsteady Natural Convection Problems

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Key Words: Topology optimization, Lattice Boltzmann method, Natural convection, Unsteady problem, Parallel computing

Natural convection is a thermal-fluid phenomenon driven by buoyancy force and widely investigated from numerical and experimental aspects. Among the previous works, mathematical optimization concerning natural convection is recognized as an important research topic for designing high-performance cooling systems such as heat sinks, energy storage devices, etc.

Topology optimization for natural convection is a relatively new and undeveloped research topic since Alexandersen et al. [1] have pioneered it in 2014. One of the difficulties of natural convection is treating the two-way coupling; fluid and temperature fields interfere. Hence, numerical simulation of natural convection is typically more challenging and needs higher computational cost under the same degree of freedom as forced convection. Consequently, research on topology optimization for natural convection is still limited; especially, large-scale unsteady natural convection is an open research problem.

To tackle unsteady natural convection problems, we propose a topology optimization method based on the previous work [2], in which the lattice Boltzmann method (LBM) is employed for solving forward and adjoint problems based on the so-called adjoint LBM. The LBM is suitable for solving fluid flows with parallel computing; additionally, many researchers have demonstrated the LBM can be applied for large-scale natural convection. So far, since any LBM-based topology optimization has not been proposed, even the steady-state, we first validate the proposed method via topology optimization for a steady natural convection problem as with the previous work [1]. We then demonstrate the efficacy of the proposed method through numerical examples of 2D and 3D unsteady natural convection problems.

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Topology Optimization of 3D-Welded Frame Structures with regards to Manufacturing Cost

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Key Words: Manufacturing cost, Topology optimization, Welded frame structure

Manufacturing cost is seldom considered in the topology optimization of structures, which is often based solely on structural criteria and weight. Consequently, the optimal design may exhibit superior mechanical performance but be costly to manufacture. While the amount of material in a structure may contribute significantly to its cost, there are also other costs associated with the fabrication process. In the case of the welded frames considered in this work, for example, the manufacturing cost is influenced by the cost of cutting, welding and painting frame members.

Ground structure methods have been used to minimize the manufacturing cost of truss structures. In these methods, which use 1D-elements to represent the structure and for analysis, it is easy to compute costs associated with, for example, the length of the truss elements and the number of struts. However, other cost components, such as the cost of welding, cannot be readily computed because they require a calculation of the welding length, which is difficult to compute from the 1D-representation. Moreover, the structure must be a topological subset of the initial design (the ground structure), thus they cannot model arbitrary topologies. Some density-based topology optimization techniques for continua consider the manufacturing cost of additive manufactured components. For these manufacturing processes, it is possible to express the manufacturing cost in terms of quantities that can be computed from the field representation, such as surface area and the volume of the support material.

We propose a method for the topology optimization of welded frame structures with regards to manufacturing cost. The frame is modeled as the union of 3D-primitives. The analysis is performed on a fixed finite element mesh as in density-based methods. To represent the frame using primitives but still perform the analysis on a fixed mesh as in density-based methods, we employ the geometry projection method. In this technique, the geometric parameters of the primitives are mapped onto a density field that is subsequently used to interpolate material properties, just as in density-based methods. The proposed approach has several advantages. Each term of the manufacturing cost function of 3D-primitives can be computed directly in terms of the geometric parameters of the primitive or through the projected density. The geometry projection mapping is differentiable, hence we can use efficient gradient-based methods for the optimization. Re-meshing is circumvented. We present examples of 3D-truss and plate frame designs with minimized manufacturing cost subject to a maximum displacement constraint.

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Topology Optimization of Duplex Structure considering Interface Debonding

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Key Words: *Multi-material, Topology optimization, Interface property, Interface thickness, Finite strain*

Multi-material design is known as one of effective ways to achieve a lightweight and high strength structure. Recently, computer-oriented design approaches have been applied to multi-material structure design [1, 2]. In a multi-material structure, the stress and strain are localized along the interface between different materials. However, the interface is generally assumed as perfect bonded in these design approaches.

In this study, a computational design method of duplex structure considering interface strength was proposed based on topology optimization method using level-set function [3]. A simple interface debonding model based on maximum principal stress was integrated into an implicit nonlinear finite element method at finite strain. Here, the interface was described as finite volume region centred on the boundaries between the two materials using a distance function. In topology optimization, a standard topological derivative based on adjoint variable method was employed for the update of the structure in consideration of the debonding state at previous iteration. Numerical demonstrations were performed to present the applicability.

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Topology Optimization of Finite Strain Dynamic Structural Problem

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Key Words: *Topology optimization, Dynamic structural behavior, Finite strain, Stabilization*

The present study addresses topology optimization of finite strain dynamic structural problem with a volume constraint. The difficulty in topology optimization considering both dynamic structural behavior and finite deformation may be how to define/formulate the physically understandable and appropriate objective function and how to deal with severe mesh distortion of low density elements. Furthermore, convergence to the optimal solution deteriorates, remaining the grayscale in the final layout.

In this study, we assume a problem setting that the structure is subjected to a temporal dynamic load and then put the structure in a state of free vibration after the load released. To stabilize the structural analysis, the interpolation scheme for fictitious domain techniques by Wang et al. [1] is applied.

Firstly, the time integral of the squared nodal displacement at the target point is chosen as the objective function. Secondary, mean compliance is chosen as the objective function and the optimization results are compared with those of the first objective function. Finally, the characteristic problems in topology optimization of finite strain dynamic structural problem are discussed through a series of numerical examples.

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Topology Optimization of Piezoelectric Energy Harvesters for Output Power under Harmonic Loads

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Key Words: *Topology optimization, Piezoelectric energy harvester, Output power, Polarization directions, Harmonic loads*

Output power and operational bandwidth are the two most important metrics for piezoelectric energy harvesters (PEHs) in practice. Upon literature, previous researches on topology optimization for PEHs are mainly limited to energy conversion efficiency enhancement, while much less attention has been given to the output power. This work proposes to enhance the output power by simultaneously optimizing the topological distribution of piezoelectric materials and their polarization directions. A finite element model subject to harmonic loads is particularly established, which is capable of accounting for both PEH design and external electrical resistance. To facilitate the use of gradient-based mathematical programming algorithms, the adjoint method is adopted for sensitivity analysis. Numerical examples show that the proposed method can effectively enhance the output power by simultaneous designing the piezoelectric materials and polarization directions. The effectiveness of the design results has also been further calibrated by their CAD (computer-aided design) reconstructed designs with smooth and clear boundaries.

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Topology Optimization with Spatially Varying Length Scale

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Key Words: *Topology optimization, length scale, density filter*

Topology optimization (TO) is a widely used computational design method for achieving an optimal structure for a given design statement. The problem includes an objective that needs to be minimized, such as weight or cost, considering a few constraints, such as allowable stress and deformation. The method updates the design iteratively using the design sensitivities of the objective and constraints. For some optimization problems, the optimized structure may include thin members that might not be manufacturable. The most common tool for constraining the length scale of structural features is by using a filter, much like in image processing, which enforces a minimum length scale on the structure. In density based TO, the filter essentially averages material densities in the vicinity of each design point and its size is considered an input parameter.

The main purpose of the proposed research is to extend the basic formulation of TO such that the minimum length scale is a design variable, alongside the pointwise density. This extension can provide many advantages compared to traditional formulations, for example: avoiding stress concentrations by local increase in length scale; and reducing manufacturing costs by forming a structure with constant length scale, that can be milled with a minimal number of tools.

Controlling the length scale of the optimized structure will be achieved by applying a PDE filter. This filter utilizes the FEM solution of a Helmholtz-type PDE to generate the filtered densities from the underlying mathematical densities that are the design variables in density based TO. The PDE filter approach is computationally more economical than the more common discrete filter. At first, the length scale parameter of the PDE filter is introduced as a single design variable, allowing the optimizer to find the best minimum length scale that is constant in space. Later, we treat the minimum length scale as a continuous field that is represented by distributing design variables throughout the design space. This enables us to tackle several problems that consist of opposing functionals, such as: maximum stiffness versus minimal stress concentrations; and maximum stiffness versus minimum size variability.

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Adaptive Multi-Fidelity Surrogate Model Assisted by Gaussian Process Regression for Design Optimization of Variable Stiffness Composites with Fiber Steering Constraints

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Key Words: *Variable Stiffness Composite, Multi-Fidelity Surrogate Model, Optimal Design*

Because of their superior mechanical properties, variable stiffness composite laminates with spatially varied orientation angles have gained widespread attentions from academic and engineering communities. To accurately model the spatial variation characteristic, a finite element model with refined meshes is required, resulting in high computation consumptions and making the design optimization quite changeling. Thus, optimization techniques based on surrogate models have been developed to relieve the high computation burden; however, as they rely on high-fidelity models with refined meshes, high computational resources are still involved and the information in low-fidelity models with coarse meshes are neglected. For this reason, studies with multi-fidelity surrogate models have been conducted to further reduce the computational costs, but neglecting fiber steering constraints and making the result not manufacturable. The present work is dedicated to presenting an efficient methodology based on adaptive multi-fidelity surrogate models for variable stiffness composite optimization with manufacturing constraints.

In this study, datasets consisting of many cheap low-fidelity analysis models and a few expensive high-fidelity models are sequentially sampled in the feasible design space with the use of a distance-based criterion. Multi-fidelity surrogate models are subsequently constructed assisted by Gaussian process regression; the optimization problem is solved employing the genetic algorithm, where the initial population is randomly produced in the feasible region and the fitness function is built with a penalized term of fiber steering constraints. The solution from the genetic algorithm is selected based on the distance infill criterion to adaptively update the multi-fidelity surrogate model. The above processes are sequentially executed until the convergence criteria are satisfied. When establishing the multi-fidelity surrogate model, three types of surrogate models are newly proposed, i.e. an exponential correction function, a hierarchical Gaussian process regression with shared datasets, and a hierarchical Gaussian process regression with non-shared datasets, and compared with two classical types of surrogate model, i.e. an additive correction function and a multiplicative correction function. The proposed optimization strategy is applied in cases studies of a composite plate and a composite cylinder, and optimization results demonstrate that the developed framework calls for significantly less computational consumption. Accordingly, a novel framework for variable stiffness composite optimization with fiber steering constraints based on an adaptive multi-fidelity surrogate model is proposed and its efficacy is demonstrated.

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Considering Failure in a Concurrent Topology and Composite Laminate Optimization by means of a Gradient-based Algorithm

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Key Words: Topology, Anisotropy, Composites, Optimization, Strength

The aim of topology optimization is to define an optimal material distribution for a prescribed load case. Nonetheless, this material distribution is influenced by the considered material properties. It was demonstrated that for compliance minimisation, the simultaneous optimization of material distribution and material orthotropy results in improved yet less bulky solutions [2]. However, the optimization algorithm used by Ranaivomiarana *et al.* [2] is limited to only compliance minimization. Furthermore, strength considerations should be included for a more relevant industrial application, and require the use of a gradient-based algorithm, such as done in [1]. Therefore, whilst taking advantage of the simultaneous anisotropy optimization with the inclusion of strength constraints, a novel topology optimization approach is first proposed. This entails a gradient based topology optimization, with the concurrent consideration of anisotropy and compared to the results of Ranaivomiarana *et al.* [2] for validation. The suggested method is constructed on the adequate combination of approximation in the Methods of Moving Asymptotes algorithm class [3] based on the nature of the variable. The polar formalism is used to characterize the anisotropy, which is limited to the space of composite laminates by means of the geometric bounds [4]. With similar results for compliance minimization, strength considerations are being included in the optimization structure. Failure will be considered by means of an anisotropic failure envelope, and aggregated into a single value in order to improve computational cost. This method was shown to be effective by Mirzendehdel *et al.* [1]. This framework will also be used for the further incorporation of buckling constraints. This research project is funded by STELIA Aerospace.

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Extended Level Set Based Multi-Material Topology Optimization Method Using Reaction-Diffusion Equation, Applied to Elastic and Thermal Problems

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Key Words: *Extended Level Set Method, Topology Optimization, Multi-material*

Topology optimization is one of the most flexible design methods among structural optimization methods, and it is capable of drastic improvement without depending on the initial structure, so it is expected to be very useful in engineering applications. On the other hand, in order to satisfy the required functions and cost constraints of a mechanical system, it is necessary to select materials with appropriate properties according to the application and to arrange them appropriately. Therefore, research on multi-material topology optimization methods that extend the framework of topology optimization has been actively conducted.

In this study, we propose a new multi-material representation method, the extended level set method. In this method, the level set method in two materials, is generally extended. Proposing method uses the same number of level set functions, as the number of possible phase changes in multi-material topology optimization, i.e., the number of combinations to choose two materials from among those used. The existing methods use only a smaller number of level set functions, which leads to complicated design sensitivity and high initial structure dependence.

First, we explain the formulation of the proposed method. Then construct a multi-material topology optimization method based on the new material representation method. After that, the numerical implementation method is described. Finally, numerical examples of the method applied to elastic and thermal problems are given to demonstrate the usefulness of the method. In the numerical examples, reasonable results were obtained not only for the usual stiffness maximization but also for the compliant mechanism design problem. It was also applied to the problem of maximizing thermal diffusion in a system with internal heat generation, which has few examples in multiple materials, and reasonable results were obtained. In addition, it was shown that the geometric complexity can be controlled for each combination of two materials.

We believe that this method will become one of the key concepts in multi-material topology optimization. Based on this method, the multi-material topology optimization method will be applied to a variety of mechanical problems. In addition, this method may also be applied not only to topology optimization, but also to various other fields of numerical computation that deal with multiple spatial domains.

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Integrated DIC Based Identification of Local Elastic Properties of Discontinuous Long-Fiber Composites

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Key Words: Digital Image Correlation, Inverse Problems, Composite materials, Finite Elements Method

We present a novel application of integrated digital image correlation to the identification of spatially variable elastic fields, applied to Discontinuous Long-Fiber (DLF) composites.

DLF composites such as carbon fiber sheet-molding compounds (CF-SMC) show good potential as a substitute to metal parts in the automotive industry due to their high specific stiffness and low-cost manufactiring process. However, the use of long fiber bundles leads to a microstructure with no scale separation, resulting in variable mechanical properties at the scale of a part. Common approaches to characterize DLF compostes rely on micromechanics simulations based on synthetic microstructures, generated from various chips packing algorithms that, in some cases, model the fibers flow and reorientation during the molding process [1]. These methods, although useful for estimating the macroscopic properties of DLF parts, show no application for identification of mechanical properties of specific parts.

Digital Image Correlation (DIC) is a common technique to measure the strain field of a material sample under loading. Digital twinning tensile tests have lead to the so called Integrated DIC (I-DIC) method, and was successfuly employed to identify parameters of non-linear constitutive laws, by minimizing the simulation to experiment gap [2]. In this work, we extend the I-DIC method to the identification of spatially varying elastic fields. Our main contribution is the identification of fields in a high dimensional space. As opposed to common application, approximating the parameter of interest sensitivity fields with finite differences is intractable, and we resort to an adjoint-based inverse problem formulation with proper regularization. Our method also recovers the experiment uncertainty parameters, such as non-uniform boundary conditions and rigid body motions. The identified elastic field of interest allows further mechanical simulation to identify local weak spots under a given loading. To the knowledge of the authors, this is the first time that non-constant elastic fields are recovered from real data.

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Shape Optimization of Cellular Structures Using a Reduced Order Model

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Key Words: *Reduced Order Model, Finite Element Analysis, Shape Optimization, Lattice Structures*

Micro-architected cellular structures are defined as large macroscale structures composed of unit cells. One variety of such structures are truss lattices, which are comprised of, e.g., octet truss unit cells. The fabrication of micro-architected cellular structures at fine scales over large volumes has been enabled by recent advances in additive manufacturing. Consequently, the need for accurate and efficient analysis and design optimization of these structures has increased considerably. Homogenization methods, which replace a detailed model of a unit cell with bulk properties at the macroscale, are quite popular for the simulation of cellular structures [1]. However, in practice, these approximations are often employed beyond their range of validity. On the other hand, it is costly to simulate large cellular structures using a fully resolved finite element analysis; particularly in an iterative design optimization context that requires many such simulations.

To balance accuracy and cost, we utilize a Reduced Order Model (ROM) that models the deformation of a complex unit cell structure as a type of super element [2]. Specifically, a fine-scale conformal FEM mesh of the unit cell is mapped to a single, high-order element, and the stiffness matrix of this element is computed using ideas akin to influence coefficients. The influence coefficient displacement fields serve as the element interpolation functions, rather than the usual shape functions. This technique also guarantees displacement continuity throughout the macroscopic structure, even when neighboring unit cells have dissimilar structures. Furthermore, increasing the order of the super element will yield greater accuracy. To demonstrate the performance of the proposed ROM method, we compare it against fully resolved FEM simulations of large cellular structures. Our numerical experiments show that the ROM solution converges to the fine-scale solution as the ROM order is increased.

Finally, we explore the suitability of this method for parameter-based shape optimization. In our approach, the internal characteristics of the unit cells, e.g., the thickness of the rods in truss lattices, serve as design variables. We interpolate the ROM stiffness matrix at any point in the design space using geometric mappings and machine learning. A small set of matrices for different unit cells are computed *a priori* to feed into our ML interpolation algorithms. In the optimization, we minimize the macroscopic structure's compliance subject to a constraint on its mass. We compare our results against traditional density-based methods with homogenization.

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Topology and fiber orientation optimization of variable-stiffness composites using lamination parameter interpolation

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Key Words: Topology Optimization, Fiber Orientation Optimization, Composite Plates, Lamination Parameters, Variable Stiffness

In the last decades, composite materials have gained increasing interest in many industrial applications due to their advantageous mechanical properties. In addition, thanks to the recent improvements in manufacturing technologies, the fibers within the laminate can be curved to further improve performance by achieving variable-stiffness characteristics. However, in the design of variable-stiffness composites, complicated procedures are required to maximally utilize the tailoring potential while ensuring the manufacturability. The structural performance of laminates can also be enhanced through topology optimization techniques, which are mainly implemented for isotropic materials and are more recently extended for constant-stiffness composites [1]. This study addresses the optimization of both laminate topology and fiber orientation by combining moving morphable components [2] and the lamination parameter interpolation method [3] for efficient parametrization of the material layout and stiffness directionality, respectively. The topology of the structure is first optimized by assuming isotropic material properties. Then, to curb the problem dimensionality and to ensure a smooth distribution of fibers on the laminate, master nodes are placed on the key points within the optimal topology. Finally, the optimal lamination distribution in the part of the domain occupied by material is determined through distance-based interpolation. Multiple static test cases have been considered to demonstrate the applicability of the proposed approach. Since the optimization is carried out by using black-box optimization techniques, this study represents a good basis for crashworthiness applications, where the objective functions are highly multimodal and gradients are not available.

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A structural optimization strategy with micro-architectured materials and uncertainties

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Key Words: Multiscale, Multiphysics Problems, Uncertainty propagation

Topological optimization is an example of a design that is based on the use of numerical simulation to predict the performance of a structure that does not yet exist, but whose sizing is to be guided. These approaches belong to the so called inverse many-query problems (such as uncertainty propagation) which make many calls to the direct problem of predicting the performance of a given structure. This direct problem must therefore be able to be solved at low computation cost.

In the case where micro-architectural materials are used (for example heterogeneous materials whose microstructure is made up of several phases), and with additive manufacturing techniques such as 3D printing, the microstructure (geometry and / or phases) can also be optimized on a small scale. Effective techniques must then be put in place to avoid the explosion of computational costs. Another objective is also to ensure manufacturability, with constraints on the feasibility of the microstructure. In addition, manufacturing technology needs to consider the variability in production.

We are here concerned by thermo-mechanical problems (we restrict ourselves to simplify cases of coupled linear behavior), A pseudo-periodic homogenization technique is used to understand the multiscale aspect (an additional constraint will therefore be to verify the conditions of pseudo-periodicity of the microstructure). Topological optimization is used at the macroscopic scale only, the microstructure being parameterized so as to be able to restrict the allowable (manufacturable) range of the optimization parameters of the microstructure. A previous approach was to build an abacus of macroscopic characteristics in the offline phase [2], which may turn out to be a phase expensive.

The target optimization problem is of the multiscale, multiphysical and potentially robust type. The computational cost is controlled by the use of polynomial chaos methods for the propagation of uncertainties and micro-macro substitution models [1].

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Identification of a Phase Field Model for Brittle Fracture in Random Heterogeneous Elastic Media

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Key Words: Phase field model, Brittle fracture, Statistical inverse problems, Random heterogeneous elastic media

Within the framework of linear elasticity theory and fracture mechanics, this work deals with the statistical identification of a phase field model [1] for brittle fracture in random heterogeneous elastic media. Such a phase field model is typically parameterized by the critical energy release rate (or fracture toughness) and the regularization length (describing the actual width of the smeared crack representation) which are considered as deterministic and homogeneous parameters to be identified. We consider a random heterogeneous material for which the apparent elasticity properties at a given mesoscale are modeled as a non-Gaussian tensor-valued random field [2].

The identification of the fracture properties of a cracking heterogeneous elastic material requires solving a challenging statistical inverse problem. An identification method with an *ad hoc* cost function is specifically developed for solving this statistical inverse problem. The performances of the proposed identification method are illustrated on a classical benchmark problem for brittle fracture.

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15th World Congress on Computational Mechanics (WCCM-XV)
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On the Design of Artificial Neural Networks for solving Statistical Inverse Problems in Computational Biomechanics

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Key Words: Identification, Statistical inverse problems, Artificial neural networks, Biomechanics

This work deals with the statistical inverse identification of geometrical and mechanical properties of a biological tissue (cortical bone) using artificial neural networks (ANNs). The stochastic computational model (SCM) corresponds to a random elasto-acoustic multilayer model [1] for the ultrasonic characterization of cortical bone properties with the axial transmission technique. It allows for simulating the propagation of ultrasonic waves through a three-layer biological system made up of two deterministic homogeneous acoustic fluid layers (soft tissues and marrow bone) surrounding a random heterogeneous elastic solid layer (weaken cortical bone). A probabilistic model of the random elasticity field is introduced to take into account the uncertainties induced by the experimental configuration. The input hyperparameters of the SCM are the thicknesses of healthy and weaken parts of cortical bone, a dispersion parameter controlling the statistical fluctuations of the random elasticity field, and a spatial correlation length along the thickness direction characterizing the spatial correlation structure of the random elasticity field. The output quantities of interest of the SCM are the scattered acoustic energies stored at 14 receivers located inside the soft tissues layer. The statistical inverse problem related to the identification of these hyperparameters from given quantities of interest may be solved using classical stochastic optimization algorithms that usually require many calls to the SCM, thus resulting in a high computational cost. Alternatively, an ANN-based identification method [2] is proposed here and applied to the identification of the hyperparameters from the quantities of interest of the SCM. An initial database is first generated by using forward simulations of the SCM and allows a dataset of hyperparameters and quantities of interest to be collected. A processed database is then constructed by conditioning the hyperparameters with respect to the quantities of interest using classical kernel density estimation methods for improving the ANN performance. A multilayer ANN is finally designed and trained from the processed database to learn the nonlinear mapping between the quantities of interest (ANN inputs) and the corresponding expected mean value of the hyperparameters (ANN outputs). Lastly, the trained ANN can be used to directly perform the identification of the hyperparameters from given quantities of interest.

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Semi-supervised deep learning of constitutive relations

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Key Words: Constitutive relations, semi-supervised learning, deep learning, neural networks

Nuclear fuel performance codes, developed in the framework of the PLEIADES platform, require the description of complex nonlinear mechanical behaviors able to represent the microstructural evolutions of the materials under irradiation [3]. Therefore, modeling the constitutive relations is a major hurdle in order to perform mechanical computations. In this work, the constitutive relation is replaced by a neural network model, as proposed in [1]. The method has three advantages: explicit formulation of the constitutive equation is *not required*, the approach is *non-intrusive*, and the *tangent operator is directly available* thanks to automatic differentiation mechanisms implemented in modern deep learning libraries.

Different neural network models trained on synthetic datasets are presented. First, we approximate a parametric nonlinear elastic material with a deep feedforward neural network, then a history dependent material with a recurrent architecture.

Data augmentation strategies are discussed in order to tackle small labeled datasets. Moreover, the numerical stability of the computations is improved by considering constraints during the learning phase. These constraints are taken into account using two different methodologies, via the neural network architecture [4] or using a semi-supervised learning approach. The latter consists in combining a *small* labeled dataset of *strain-stress* samples with a *large* unlabeled dataset of *strain only* samples to train the model.

Finally, the methodology is applied to toy examples using the PyTorch deep learning library, the MFront material knowledge tool [2], and the FEniCS finite element platform.

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A novel functional structure with compression-torsion bistable by bi-material 3D printing

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Key Words: *Additive manufacturing; Bistable; Compression-torsion; Mechanical metamaterial*

Bistable structures have two stable equilibrium states in the absence of external loadings. They have been widely used in the applications of actuators, energy absorbing, precise motion control and reconfigurable structures[1]. To date, most designed bistable structures can achieve either uniaxial deformations under axial loads or torsions under torsional loads[2]. The remained open questions are that how to design the structures to achieve an extended type of deformation modes[3].

Here, we create a novel structure configuration, which realizes torsional bistability subjected to uniaxial compressive loads. The geometry of the structure is combined by two twisting chiral frame structures, which have opposite twisting modes under the same compressive loadings. In order to achieve bistability, some struts are composed of two materials which have different stiffness. By carrying out a parameter study, various compression-torsion bistable structures have been made. Furthermore, the designed compression-torsion bistable structures can be made as lattice structures and acquire multi-stability. Last, the bi-material structures are manufactured in an integrated manner by using the Stratasys® J750 3D printer. Our study provides new deformation modes and deformation mechanisms of bistable structures, and it's the first time to realize torsional bistable deformations under compression load.

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Design of Metastructure for Piezoelectric Energy Harvesting via Isogeometric Shape Optimization

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Key Words: Energy Harvesting, Isogeometric Analysis, Mechanical Metamaterials, Piezoelectric, Shape Optimization, Vibrations

With the rapid development of Internet of Things (IoT) technology, worldwide efforts to seek continuous energy sources for various information sensing devices remains critical. A meritable pathway to mitigating environmental degradation is to investigate and innovate more effective renewable energy solutions that capitalise on the natural phenomena around us. Energy from mechanical vibrations provides a sustainable source that accelerates the renewable energy movement. Vibrational Energy Harvesting involves converting mechanical energy available in the environment into electrical power. Piezoelectric Energy Harvesters (PEHs) stand out over other methods due to their higher efficiency per area unit. However, scalability is their main challenge due to low energy generation and poor sensitivity to aperiodic and broadband vibrations. This study investigated the Shape Optimization of metamaterial-inspired structures to improve voltage generation. The device design consists of a periodic cells array which induces local resonance inside the structure. Here, PEHs are modelled according to the Kirchhoff-Love Plate theory and solved numerically with Isogeometric Analysis. Nitsche's Method has been used to couple multiple unit cell patches, creating a PEH plate. Comparing experimental results and the IGA solution verifies PEH dynamic behaviour from model predictions. By investigating the frequency response functions of PEH plates composed of different cell geometries, variations in metastructure designs to improve voltage output when exposed to low-frequency vibrations are studied. Developing high-performing PEHs will provide a promising pathway for manufacturing versatile piezoelectric harvesters and sustainable monitoring devices for IoT technology.

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Effective Stiffness, Strength, Buckling and Anisotropy of Foams Based on 21 Triply Periodic Minimal Surfaces

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Key Words: *Cellular Materials, Effective Properties, TPMS, Finite Element Analysis*

The study of cellular materials, especially triply periodic minimal surfaces (TPMS) and their properties has gained considerable significance in the recent years due to the advancement in additive manufacturing technologies. In this study, 21 TPMS architectures are studied by comparing their effective stiffness, strength, buckling and anisotropic properties. The TPMS lattices are generated using level set equations where the relative density of each lattice is varied to study the effective properties as a function of relative density. Finite element models of these lattices are built to study the deformation behaviour under uniaxial, shear, hydrostatic and buckling loading conditions. Effective properties such as Young's modulus, shear modulus, bulk modulus, Poisson's ratio and strengths under uniaxial, shear, hydrostatic and buckling loading are computed and compared against each other and other common lattice structures[1]. In addition, anisotropic behaviour as well as the orientation dependence of the properties of each lattice are also studied. The geometric efficiency criterion is predominantly used to evaluate the different structures and the results obtained are consolidated in both quantitative and qualitative manner. Gyroid, Y and C(Y) lattice structures have the least geometric efficiency at both low and high relative densities, even though Y lattice shows higher than normal shear stiffness. The FRD, OCTO, Batwing and IWP lattices show good overall promising geometric efficiencies for most of the properties. In fact, most of the existing literature on investigating the mechanical properties of TPMS lattices and employing theme for enhancing structural efficiency has been focused on the Gyroid lattice. It is shown in this study that other lattices (e.g., FRD and IWP) are much more promising to be further investigated and employed for various structural applications. Also, Primitive lattice is highly recommended for structural applications where shear stresses and deformations are dominant such as sandwich panels. LACE (Lattice Architectures for Cellular Engineering), an open-source software which runs on MATLAB runtime library was developed to design complex TPMS architectures. LACE gives the end user the flexibility to generate intricate geometries that meets the strength and stiffness requirements for any application. The effective properties database together with LACE provides a robust framework for solving a wide range of engineering design and optimization problems.

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Frequency-adaptable Elastic Metasurface with Multiple Functionalities

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Key Words: *frequency-adaptable, metasurface, phase shift, FEMs*

A metasurface is a two-dimensional metamaterial that possesses remarkable wave manipulation properties by controlling the wavefront arbitrarily. Based on the concept of generalized Snell's law, a metasurface could achieve any desired phase profile that covers the full 2π phase span. Nevertheless, most conventional metasurfaces are limited to permanent functionalities or working frequencies once manufactured. This hinders their applications in intelligent systems, as well as in application scenarios embedded in sharply changeable environment, which may cause their working frequency shift or even make them fail. To overcome this disadvantage, we propose an adaptive elastic metasurface composed of piezoelectric stacks to manipulate elastic longitudinal waves with high transmission performance at different frequencies. In this study, piezoelectric stacks are connected to shunted negative capacitance circuits to realize multiple functionalities without changing the structure of the metasurface. Through proper tuning of the negative capacitance in the shunting circuit, the effective modulus of the metasurface units could be tuned continuously, which enables the metasurface to produce local phase shift cover 0 to 2π range. Both analytical model and numerical simulations are developed to obtain the corresponding negative capacitances. Furthermore, computational method is used to study the effect of negative capacitances on transmission and phase shift of the waves in broadband frequencies. The proposed metasurfaces are simulated based on FEM to illustrate the functionalities, such as anomalous refraction, wave focusing and nonparaxial propagation at different frequencies, which can be easily performed by tuning the negative capacitance.

Hierarchical Isotropic Microstructures

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Key Words: *Microstructure, Isotropy, Hierarchical microstructures, 3D-printing*

Isotropic microstructures have identical stiffness along all directions, and they are widely used in engineering applications. Up to date, a various number of isotropic microstructures have been designed. For instance, 2D hexagonal and triangle microstructures are isotropic in plane. In 3D, a family of combined isotropic microstructures has been designed[1,2], which combines two or three elementary microstructures (i.e. simple cubics, body-centred cubics and face-centred cubics) in a right proportion. Besides, another family of quasiperiodic *n*-fold microstructures is identified to achieve isotropic stiffness[3]. Both theoretical proofs and numerical results have proved that the above two families of microstructures are able to attain the stiffness upper bounds in theory in the case of low density limit. More isotropic microstructures can also be designed by using the topology optimization technology[4].

Here, we present a novel category of isotropic hierarchical microstructures (Iso-HMs). These Iso-HMs are built by incorporating second-order microstructures into the solid regions of the first-order orthotropic microstructures. The underlying concept to achieve isotropy is to identify the right second-order microstructures that have complementary directional stiffness with respect to the first-order ones. That is, in the direction of the highest stiffness for the first-order microstructure, the second-order microstructures have the weakest stiffness, and vice versa. Several examples are presented based on the square unit cell with rectangular central holes in the first-order, wherein the crossing type microstructures are employed in the second order. By using such a design methodology, various isotropic hierarchical microstructures are obtained. It is observed that the isotropic stiffness is between the highest and lowest directional stiffness of the first-order microstructure. Also, the hierarchical microstructures have higher buckling strength than the original first-order microstructure. We will also show that by using a high-resolution PuSL 3DP technology, these Iso-HMs can be fabricated. The samples have minimal 50um features and the ratio between the maximal and minimal feature sizes reaches over 1000:1. Such a design framework could help identify a wider range of microstructures that have superior stiffness and strength, and also multi-functionals.

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Intracranial Acoustic Field Optimization of a Point-Like-Scatterers-Arrayed Transcranial Lens

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Key Words: Fresnel Lens, Point-like Scatterers, Optimization, Integral Equation, Transcranial Focusing

In order to promote the effect of a thrombolytic agent as a non-invasive cure for the cerebral infarction of an acute stage, a real-time adaptive ultrasonic lens constructed by arranging point-like scatterers on a lattice has been proposed according to the concept of Fresnel lens. The structure was optimized from the initial arrangement of the scatterers.

The dependence of convergence of optimization on the initial state and on the thickness of lattice has already been investigated. Four kinds of the initial states was considered, that is, the holographically generated configuration, the configuration without the scatterers on all of lattice points, the configuration with the scatterers on all of lattice points and the configuration with the randomly distributed scatterers. It has been found that the initial configuration without the scatterers shows the fastest convergence and increase of the number of layers improves the ratio of the power of the ultrasound wave at a focal point to that of the background. The convergence of optimization for three kinds of thickness, that is, the number of layers has also systematically investigated.

The proposed lens constructed by optimally arranged point-like scatterers on a lattice has showed superior performance focusing the incident plane wave on a focal point and suppressing the sound field except the vicinity of the focal point. In the present study, we have investigated the transcranial focusing performance of the point-like-scatterers-arrayed lens. The purpose function is defined as the sound field vanishes within the skull except the focus(es) and becomes higher at the focus(es) than around. The placement of the point-like scatterers is optimized in terms of the purpose function. It has confirmed that the lens focused the incident plane wave with enough intensity even transcranially.

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Multiscale Optimization of Resonant Frequencies for Lattice-Based Additive Manufactured Payload Interfaces

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Key Words: *Multiscale Optimization, Resonant Frequencies, Additive Manufacturing, Lattice*

In this work a novel method of resonant frequency optimization is demonstrated using a multiscale, functionally-graded metamaterial optimization approach to predict and alter the structural and dynamic properties of an additively manufactured lattice structure. The ability to tailor resonant frequencies of structural components offers much greater design freedom for engineers and offers savings in weight and cost alongside the improved resonant properties. The metamaterial used is a 7 member, open-truss lattice with spatially varying truss radii capable of producing a functionally graded lattice structure [1].

The work employs multiscale methods using homogenization of structural properties of the unit cell dependent on the radii of its 7 members. This is achieved by determining homogenized material properties using finite element analysis (FEA) of the microscale structures subject to periodic boundary conditions. This approach is implemented in the open source, python based FEA solver, FEniCS. These simulations are used to determine the homogenized stiffness of the unit cells in the 3 principal directions and 3 shear terms as well as the lattice volume fractions. This database is then used to fit a series of 7th-order polynomials which predict the homogenized material properties based on the lattice parameters of each unit cell. During macroscale optimization the member radii are used to evaluate the material properties of the macroscale finite elements and hence evaluate the global resonant frequencies and volume fractions.

For the macroscale optimization an interior point algorithm is employed using the open source optimization software IPOPT. In this approach the truss radii represent the design variables of the optimization and the objective is the tailoring of resonant frequencies subject to volume constraints. The inclusion of a modal tracking algorithm allows for the optimizer to track resonant modes based on their mode shapes rather than frequencies. This method allows for the order of resonant modes to be changed during optimization as well as preventing localized mode shapes from interfering with the optimization process.

The work has been demonstrated through optimization of a Payload Attach Fitting (PAF) used to attach payloads to a spacecraft. The interface can be used to drastically alter and optimize the resonant frequencies of the combined PAF and payload structure. Using this multiscale optimization approach allows increased versatility, lower mass and improved resonant properties without increasing design cost. The final oral presentation will demonstrate the metamaterial's ability to achieve a large range of resonant frequencies as well as demonstrate excitation avoidance.

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Multiscale topology optimization for electromagnetic metamaterials by using high-contrast homogenization method

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Key Words: *electromagnetic metamaterial, multiscale optimization, homogenization method, topology optimization*

Electromagnetic metamaterials are artificially designed materials that have special electromagnetic properties induced by a local resonance in a periodic array of unit cells, such as negative permeability. Metamaterials are expected to be applied to innovative devices, for example, superlens, filtering devices, and cloaking devices.

Designing metamaterials by trial and error is difficult because the local resonance depends on the structure of the unit cell and small differences in the design affect their overall performance. One way to solve this problem is to use topology optimization for the design. During the optimization, it needs to evaluate the performance of a metamaterial, however, it takes a huge computational cost to solve the Helmholtz equation directly to obtain the wave propagation in the metamaterial. Therefore, a more efficient method is required to optimize the metamaterial's structure. To reduce the computation cost, we introduce a high-contrast homogenization method, that was proposed in the previous work [1]. This method is suitable for the optimization of metamaterials compared to the classical homogenization methods; it can be used in a wide frequency range even if the local resonance is induced in the unit cell.

In this research, we propose a multiscale topology optimization method for the design of metamaterials that incorporates the high-contrast homogenization method with a level set-based topology optimization method [2]. First, the high-contrast homogenization method is introduced for the Transverse magnetic wave (TM wave), governed by the Helmholtz equation. Next, the multiscale topology optimization problem is formulated, in which the objective function is defined with the macro scale solution of the homogenized equation whereas the microscale structures are set as design variables. We derive the design sensitivity based on the concept of topological derivative. As numerical examples, we present waveguide problems in the T-junction structure and the demultiplexer to demonstrate the effectiveness of our method.

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Negative thermal expansion metamaterials with high energy absorption properties based topological optimization and bionics design

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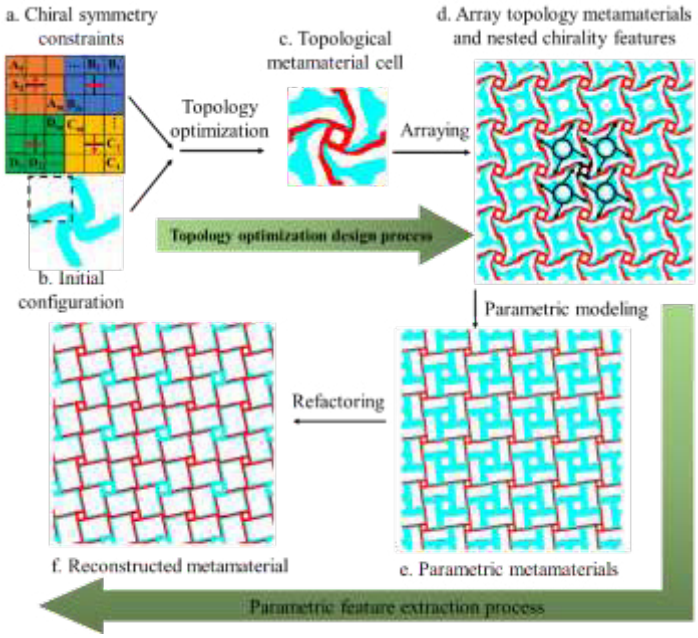
Key Words: *Topology optimization, Multifunctional metamaterial, Bionic design, Negative thermal expansion*

As the design of single-function metamaterials becomes more and more abundant, the importance of multi-function metamaterials design is gradually increasing. Among them, chiral metamaterials with compression-torsion coupling function have been widely studied because of their geometric characteristics and good energy absorption function. In this paper, we design a chiral metamaterial with negative thermal expansion and energy absorption buffering based on topology optimization. We find that topological results are nested by two chiral structures with fractal characteristics similar to biological structures. Inspired by this, and combined with bionic and typing design concepts, we further designed the chiral structure and added more layers. Numerical simulation shows that the enhanced fractal structure can effectively maintain the negative thermal expansion of the material. In addition, the experiments show that the multi-level metamaterial can restrain the large damage caused by structural fracture more effectively than the traditional single-layered chiral structure, and the property is universal to brittle and ductile materials.



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Title

Optimization of Structures with Self-supporting Enclosed Voids and Build Orientation for Selective Laser Melting

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Abstract

To compromise the manufacturability and performance for additive manufactured products, this paper proposes an alternative optimization approach to achieve rational topological designs by constraining the overhang feature only in the enclosed voids and determining the build orientation in the framework of selective laser melting technique. An identification scheme based on the algorithms in image processing is proposed to detect surfaces on the closed voids. Meanwhile, a filtering technique is employed to constrain both overhang angle and overhang height of enclosed voids. Then, the identification scheme of enclosed voids and overhang feature control are integrated in integral element-wise framework to the optimize the part topology and build orientation simultaneously. In order to demonstrate the effectiveness of the proposed approach, the popular compliance minimization problems are applied in both 2D and 3D numerical cases.

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Phononic structures for enhancing the accuracy of ultrasonic flowmeters

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Key Words: Ultrasonic flowmeter, 3D phononic crystals, wave rejection, multi-objective optimization, model reduction, additive manufacturing, ultrasonic transient experiments, Industrial Applications.

Ultrasonic flowmeters that use transit-time ultrasonic transducers face measurement errors due to "crosstalk," whereby the working signal travels through the solid region faster than the measuring fluid. Various solutions to this issue include isolating the sensor portion of the flowmeter from the surrounding, using damping systems inside the flowmeter, and attaching various resonators to the flowmeter. However, the resonators and damping systems are limited to relatively low frequencies (a few hundred kHz), and acoustic insulation becomes an issue in high-pressure environments. We propose a mounting mechanism based on a single-phase 3D phononic crystal (PnC), which can mitigate crosstalk at high frequencies (in MHz range) and thus improves the measurement accuracy. PnCs are artificial materials that possess bandgaps (BGs)—ranges of frequencies where elastic/acoustic waves are attenuated—that are generated due to Bragg scattering. We designed a PnC wave filter by engineering the BG frequency range to the working signal, and we fabricated it using additive manufacturing. Furthermore, we connected this wave filter to a transducer by using adequate mounting structures. We then verified the PnC wave filter's performance through transient ultrasonic experiments. Since the transducer is subjected to high pressures, we introduced additional objectives during the design procedure. A multi-objective constrained optimization problem to maximize both attenuation performance and mechanical strength was formulated, which was carried out via parametric optimization and sensitivity analysis. Since the finite element analysis of the entire structure is computationally intensive, we performed a model reduction at different stages of the optimization. Finally, we obtained a closed 3D PnC waveguide design satisfying both objectives.

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Robust topology optimization for thermoelastic structures with random and interval hybrid uncertainties

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Key Words: *Topology optimization; thermoelastic; robust design; hybrid uncertainties*

Considering the complex multi-physics service conditions for advanced equipment, many developments have been achieved for thermo-mechanical topology optimizations [1]. Most of these research works are focus on deterministic assumptions. However, the random and interval hybrid uncertainties related to material properties, loadings, etc. unavoidably exist in structures and may have notable influence on structural optimization [2]. A new robust topology optimization method is developed for structures under thermo-mechanical loadings considering hybrid uncertainties. Firstly, the robust objective function is defined by the lower order moments and the topology optimization model is provided under the worst case. Secondly, an efficient dimension reduction method based orthogonal polynomial expansion method is developed to calculate the statistical moments of the structural compliance, in which the multi-dimensional integrations to calculate the expansion coefficients is approximated by a series of univariate integrations. Finally, several numerical examples are provided to verify the effectiveness of the proposed method. It is proved that the robust designs have better robustness than the deterministic designs considering hybrid uncertainties.

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Topology Optimization for Pentamode Lattice Metamaterials

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Key Words: *Pentamode, Mechanical Metamaterials, Lattice, Topology Optimization*

Pentamode metamaterials are a new class of artificially engineered lattice metamaterials with vanishing shear modulus and able to support single mode of stress. In this research, a topological optimization method is first developed to generate pentamode lattices which will exibit effective material properties over a range of relative densities. The design of the pentamode microstructure is defined as a three-dimensional ground structure with at least orthotropic symmetry. Then, the necessary and sufficient condition for the elasticity matrices of pentamode metamaterials with at least orthotropic symmetry is proposed. This research shows that a large ratio between the bulk modulus and the shear modulus is not a sufficient condition for pentamode metamaterials that are not isotropic. After that, a range of new pentamode microstructures are created to demonstrate the effectiveness of the proposed design method. This study will supply a very solid foundation in princicple for application of pentamode applications, including cloaking devices.

Two-scale Concurrent Structural Topology Optimization Considering the Microstructural Connectivity

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Key Words: *Topology Optimization, Homogenization, Microstructure Connectivity*

The simultaneous optimization of the spatial distribution of multiple kinds of microstructures within a structure and their geometry configurations can effectively tailor the structural mechanical performance and enhance the multi-physics functionalities. The topology optimization technique in combination with the homogenization method have been widely adopted in such two-scale design problems. However, the homogenization-based design methods do not necessarily ensure the connectivity between different kinds of the optimized microstructures. Several methods [1-2] have been proposed to enhance the microstructural connectivity by setting up non-design domains in the microstructure based on the design experience or applying multiple optimization constraints on the microstructural boundaries.

To handle the microstructural connectivity issue, this paper proposes a microstructural connectable region method in the context of two-scale concurrent multi-material structural topology optimization. On the microscale, we parameterize the microstructural topology with the elemental relative densities, and compute their effective properties using the homogenization method. On the macroscale, we employ the discrete material optimization (DMO) method to describe the distributions of the multiple kinds of cellular materials within the design domain.

By predefining a connectable region within each kind of the designable microstructure and linking the microscale design variables therein, the connectivity between any two kinds of the microstructures is ensured naturally without applying any optimization constraints. The two-scale concurrent topology optimization problem is solved with the method of asymptotic method. This method is verified by the two-scale concurrent structural topology optimization 2D and 3D problems.

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Construction of the Education Tools for the Computer Programming - by the use of Problem Solving Environment –

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Key Words: *Programming, Education, Data Science, Society5.0, PSE,(Problem Solving Environment)*

In Japan, programming has become a important subject in elementary, junior high, and high schools in order to develop human resources who can cope with the Society 5.0 society. Data science education is also highly expected in universities.

There are many books, Internet sites, and paid workshops for learning programming in the world. When beginners learn programming, what can they expect to have learned?

There are various certifications available for this purpose. However, most of the certifications are knowledge-based, and it is a fact that they are not always practical in the real world.

Therefore, I propose a problem-solving type learning tool as an internet site.[1]
Here, if you can solve a problem, you can be considered to have learned programming.

We will prepare various problems with many examples in several languages to help the students learning.

For languages, we have so far prepared scratch, Python, and C++ [2], and we will add HTML, CSS, and PHP to them.

As for the problems, we have added access counters, bulletin boards, and the use of arrays and random numbers.

I hope that this site will help people (especially beginners) to learn programming.

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Object Classification and Segmentation Based on Deep Learning Using Underwater Mapping Data

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Key Words: *Underwater Mapping Data, AUV, ASV, Deep Learning, CNN, PointNet*

The recent development of underwater robots and measurement equipment, it has become possible to achieve high-quality underwater mapping using acoustic survey equipment with high resolution. The underwater mapping data obtained by these methods are expressed by the intensity of sound reflection and do not have color information. As a result, object identification from the acquired data depends on discrimination by professional engineer, and it is not only difficult to identify objects automatically and quickly, but also involves human error due to differences in the experience of the engineer and routine tasks.

In this presentation, a fast and accurate classification method for underwater objects using underwater mapping data obtained by a small Autonomous Underwater Vehicle (AUV) and autonomous surface vehicle (ASV) is presented. For the mapping data, in addition to underwater acoustic reflection intensity images, water depth data, point cloud data and backscattering reflection intensity data are employed. We propose the automatic classification and semantic segmentation method on deep learning using a convolutional neural network (CNN) and PointNet. In order to verify the effectiveness of the present method, we applied it to the measured several underwater mapping data.

Tsunami Evacuation Simulation Considering Building Collapse and Fire Spread

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Key Words: *Multi Agent Model, Evacuation Simulation, Building Collapse, Fire*

Japan is one of the world's leading disaster-prone countries, and has an extremely high frequency of natural disasters such as earthquakes, tsunami and typhoons. Regarding the Great East Japan Earthquake in 2011, it had been found that there is a limit to disaster prevention measures on the hardware aspects such as construction of breakwaters. And the importance of the software measures was confirmed. As one of the software measures, each municipality has been preparing hazard maps. However, hazard maps make it difficult to understand when and how to evacuate. Thus, research on evacuation simulation, which can show the above at a glance, has been widely conducted in recent years.

The present authors have also developed a tsunami evacuation system using multi-agent models. However, not only tsunami but also building collapse and fire spread have a significant impact on evacuation behaviours and survival rates of refugees as secondary damages of earthquakes.

Therefore, the purpose of this study is to develop a tsunami evacuation simulation system that considers building collapse and fire spread. The road blockage is determined by calculating the probability of road blockage due to building collapse, taking into account the scale of the assumed earthquake, the location of buildings, and the type of building [1]. For fire spread simulation, an existing simulator [2] based on the fire spread rate equation is used. Under the condition of average wind direction and wind speed in the target area, the fire spread is represented by setting any fire point and using the fire time of each building obtained by the simulation. The present system is applied to several examples to demonstrate the validity and effectiveness of the system.

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Visualization of Flow Simulation Based on AR Using GNSS Data

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Key Words: *Augmented Reality, GNSS, marker tracking,*

The visualization method for flow simulation based on Augmented Reality (AR) and Virtual Reality (VR) are becoming more powerful and popular tool for planning and design of various construction projects in accordance with the development of AR and VR technology. Focusing on AR, the AR visualization method using smartphone is attracting attention from the viewpoint of usability. The present authors have been presented a AR visualization system based on markerless augmented reality for water environmental flow problems [1]. In this system, a landscape image is used as a marker. However, this method has a problem in the stability of superimposition of CG image.

Recently, the AR using the data obtained Global Navigation Satellite System (GNSS) has been attraction attention due to the improvement of accuracy of GPS. In addition, the use of GNSS data in AR visualization has the advantage that it is not affected by the presence or absence of feature points acquired from cameras or the setting of marker locations used in marker superimposition.

This paper presents an AR visualization system for flow simulation based on AR using GNSS data. The target of visualization deals with the flow of river and sea. The present system is applied to several visualization examples to demonstrate the validity and effectiveness of the system.

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VR as an Alternative to Social Studies Field Trip - From Kinugawa Elementary School VR Field Trip

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Key Words: *VR, Full Sky Images, Elementary School, Field Trip, Covid-19,*

The spread of Covid-19, which began at the end of 2019, has led to significant changes in school education. In particular, the simultaneous closure of schools in March 2020 is still fresh in our minds, but even after that, the field of education has been subjected to various restrictions (e.g., wearing masks, dispersed school attendance, silent meals during school lunch hours, etc.).

One of the most serious cases is the cancellation of social studies field trips. The Ministry of Education, Culture, Sports, Science and Technology's Guidelines for the Course of Study (Social Studies)[1] mentions that "it is important to allow students to conduct specific research by incorporating field trips and using materials prepared by relevant organizations, according to the actual conditions of the region. This is important in terms of learning through actual experience. However, under the Covid-19 epidemic, social studies tours have been cancelled, and students have lost the opportunity to study in the field.

Therefore, with the planning and cooperation of the Ministry of Land, Infrastructure, Transport and Tourism, we created a VR tour of the Gojiri Dam and the Kawaji Dam in Tochigi Prefecture. The tour was held in November 2021 for a total of 32 fourth and fifth graders of Kinugawa Elementary School.

The purpose of this presentation is to report the outline of the VR tour and to contribute to the consideration of the use of VR in school education.

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Addressing Computational Load Imbalance in Asynchronus Distributed Contact Problems Using DARMA/vt

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Key Words: contact mechanics, AMT, load balancing

Robust contact search and enforcement is one of the more computationally intensive aspects of solid mechanics simulations. Distributed contact problems often engender a divergence between the cost of executing non-contact work versus contact work during the simulation. Implementations typically decompose mesh elements statically according to the expected load during the non-contact steps. However, the unpredictability of workloads during the contact search and enforcement step can lead to suboptimal performance with these decompositions due to imbalances that cause some processors to idle. These imbalances can be remedied by remapping contact work to other processors dynamically over the course of the simulation's timesteps.

We propose a contact algorithm that uses the dynamic load capabilities of the DARMA/vt asynchronous distributed tasking library to automatically rebalance computational loads. By exploiting the principle of persistence, we utilize instrumentation from previous time steps to load balance the current time step. This approach also accounts for migration and ghosting of elements onto processors for evaluating the contact kernels in an efficient manner. We examine several problems with a varying degree of load imbalance issues and show how our load balancing approach can improve performance significantly.

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Discretizations of high-frequency wave propagation problems on next-generation computing architectures

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Key Words: High-order, discontinuous Petrov-Galerkin, p-FEM, wave propagation

Solutions to high-frequency wave-propagation problems using traditional, low-order finite element discretizations suffer from the well-known pollution effect. Several strategies are readily available to circumvent pollution error, including high-polynomial-order finite element formulations and adapted meshes (*hp*-FEM), as well as advanced alternative discretization approaches. We concentrate on high-order continuous Galerkin FEM, as well as the discontinuous Petrov-Galerkin (DPG) method, which reduces or eliminates pollution error in numerical simulations of wave propagation problems [1]. Unfortunately, high mesh refinement and p-order required to resolve very high-frequency waves at acceptable fidelity and with minimal pollution present a challenge for ordinary computational resources. Innovations in simulation software design and increased computing power are needed to address high computational complexity and memory use.

In this talk, we look to on-node accelerators to enable high-order simulations. Graphics processing units (GPUs), with their high throughput on intensive mathematical operations, lend themselves naturally to this application. We will discuss the performance-portable discretization software tools developed as part of this work, leveraging GPU-enabled packages for high-order discretizations, linear solvers, and linear algebra operations in the Trilinos library [2]. Accuracy and performance of high-order FEM and DPG applied to the wave propagation problems of interest will also be demonstrated, investigating in detail the behavior of these methods on both conventional CPU and GPU-accelerated computers.

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Ensemble Computations on Heterogeneous Supercomputers

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Key Words: *Uncertainty Quantification, Multiphysics Problems, Multifidelity Ensemble, Task-based programming, Heterogeneous Computations*

Computer simulations are pervasive in science and engineering. Computations, together with theoretical analysis and experiments, constitute the foundation for building knowledge, whether it be to investigate a new physical phenomenon or to assess the performance of an innovative device. However, a single computation, despite its sophistication and complexity, can rarely provide sufficient and credible evidence to support a decision. To build confidence in computed outcomes, one typically conducts sensitivity analyses, investigates uncertainty, and explores design variations. All these approaches require an ensemble of computations whose results are combined rigorously via statistical analysis or optimization. In this talk we discuss the use of ensemble of simulations for multidisciplinary design under uncertainty; we have developed a novel algorithm to handle ensemble with different fidelity implemented in a new programming environment that enables the efficient use of next generation supercomputers, i.e. a hybrid CPU/GPU multimode machine. The approach is based on the Legion programming system, a data-centric task-based approach that has been shown to achieve portability and performance on a variety of modern systems (including Summit) and different complex multiphysics applications. We will present uncertainty quantification studies carried out for a solar received device and for a laser-based ignition systems using high-fidelity simulation codes written entirely in Legion. Furthermore, a theoretical framework for optimal multi-fidelity scheduling on heterogeneous computer architectures will be discussed.

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MTwin: Porting and customizing the computational mechanics solver MSolve for HPC execution in Microsoft Azure

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Key Words: *Cloud computing, HPC, Azure, Computational Mechanics, Domain Decomposition, MSolve*

Solving real-world industry problems in the field of simulation and digital twins can be really challenging in terms of computational resources. This stems, not only from the complexity and sheer magnitude of the computational models of such problems but also from the fact that the evaluation of the model response model involves the repeated solution of near-by problems, either from the evaluation of non-linear transient response and/or from the evaluation of the uncertainty response of the model [2].

Computational challenges are also present when considering multiscale analysis since the evaluation of the constitutive behavior of a material involves the solution of another detailed model. The combination of both, especially for the case where the aforementioned computational models have uncertain properties, can result in enormous computational demands that can be met only with the use of HPC platforms and algorithms.

In an effort to provide pay-as-you-go computational mechanics services where such challenges need to be addressed, NComp has utilized MSolve [1] and developed specialized HPC modules that utilize distributed parallel algorithms that harness the power of both CPUs and GPUs [3] in order to solve such demanding problems in reasonable wall clock times, relying on public cloud resources. In this work, we will describe the computational paradigms, APIs and algorithms that were used for this endeavor.

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Optimizing Open-Source CFD Software on a GPU Supercomputer

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Key Words: OpenFOAM, RapidCFD, conjugate gradient method, DIC, DILU

OpenFOAM [1, 2] is GPL licensed open-source CFD software. OpenFOAM runs as a single CPU process, but also as multiple MPI processes by applying spatial decomposition to the target domain. Studies have been reported that the software scales to thousands of CPU cores [3]. However, it does not support any accelerators such as HPC-oriented GPUs, which usually have higher memory bandwidth than high-performance CPUs.

In this presentation, we propose various techniques to accelerate RapidCFD [4], a GPU version of OpenFOAM mainly developed by SIMFLOW Technologies: 1) We propose a GPU-accelerated version of the Diagonal-based Incomplete Cholesky (DIC) and the Diagonal-based Incomplete LU (DILU) preconditioners. Our DIC/DILU implementation applies a graph-coloring algorithm to coefficient matrices to detect available parallelism on its forward and backward substitution steps. 2) We identify and resolve RapidCFD's potential performance issues that become bottlenecks on large-scale runs, including redundant memory allocation/deallocation and fragmented GPU kernels. 3) We propose an adaptive method to adjust collective communication frequency among processes during CG iterations.

We evaluate the performance of our proposed methods on the ABCI supercomputer; we achieve a 2.6x speedup than OpenFOAM on ABCI's 64 NVIDIA A100 GPUs to compute a 68 M-cells unstructured mesh. We also evaluate the effectivity of 3) under a strong-scaling configuration, resulting in a 1.6x speedup than the original code on 32 A100 GPUs. In addition, we discuss performance advantages of the two different architectures (CPUs and GPUs) for such CFD software and its future prospect.

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Performance Analysis of 3D Ground Application for Next-Generation Supercomputers

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Key Words: High-Performance-Computing, Profiling, Roofline Model, Tuning, Nonlinear Dynamic Analysis, Finite Element Method, FrontISTR, Computer Systems, 3D Ground Analysis

Understanding the current computer systems limitations and their abilities to run application programs at peak performance is an important requirement for designing the next generation of parallel architectures. A software approach relies on profiling the performance bottlenecks to uncover parts of the architecture which should be enhanced. We focus our analysis on a real application that we received from industrial users: a large-scale simulation of Kumamoto earthquake used in design innovation. This application is governed by a time marching loop (Newmark-beta) and a nonlinear loop (Newton-Raphson) nested inside. Iteratively, a discretization (FEM) builds the input matrix and a solver computes the linear solution.

Structural Analysis simulations are often memory-bound due to large matrix processing. To alleviate this problem, domain decomposition is applied on the input mesh so that multiprocessing can accelerate the computation on distributed memory. However, our analysis shows that several aspects limit the performances on both Fugaku and ABCI supercomputers. Locally, the matrix generation hotspot loops are slow down by the CPU cache hit latency and inefficient memory access. At large scale, the strong scalability is limited by the preconditioner power, a high load-imbalance affects the parallel efficiency of matrix generation and a 30% communication overhead degrades the solver computation.

In this work, we propose a series of performance tuning for the *FrontISTR* nonlinear dynamic solver based on a systematic approach which is driven by the roofline model for assessing hardware limitations of computer systems. We identified the main performance bottlenecks with profilers then we generated and located the positions of each hotspot loop kernels on the roofline model. From such insights, we applied appropriate optimizations (vector alignment, loop unrolling, arithmetic tuning, dimension exchange) and analysed the effect of various parameters (stride memory accesses, store, fma and simd instructions) to minimize the gap between kernel points and the compute/memory performance ceilings.

Our performance tuning achieved a 3x acceleration of the two main hotspot loops among others, resulting in a 1.83x speed-up of the overall stiffness matrix generation computation.

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Ratel - a Portable and Scalable Package for Solid and Fluid Mechanics

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Key Words: Multiscale Problems, Matrix-free solvers, software design, high performance computing

Ratel is a new, open-source package built on libCEED [1] and PETSc [2] capable of solving complex solid/fluid mechanics problems without sacrificing computational performance. This package provides a flexible yet intuitive user interface that reduces the prerequisite effort required for use, encouraging community involvement and development. Similar to libCEED and PETSc, Ratel is both performance portable and scalable allowing for effective material simulations on a variety of computing systems. Notably, Ratel uses single-source physics implementations with Just-In-Time compilations (rather than with domain specific languages or templates) and supports matrix-free high order elements. Additionally, we discuss high-performance automatic differentiation using Enzyme [3] to simplify the development of new material models with consistent Jacobians. We discuss Ratel's solver functionality including quasi-static and dynamic solvers and composite material support. In this presentation we also investigate Ratel's performance on CPUs and GPUs, number of nodes, and solver degree for various physical simulations taken from Ratel's example suite. Finally, Ratel is structured to support uncertainty quantification and optimization studies.

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Design of Filters Consist of Resolvents with Real Shifts for Solving Eigenpairs with Lowest Eigenvalues

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Key Words: Eigenproblem, Filter, Resolvents, Real Shifts

By using a filter, we solve a small number of eigenpairs of a real symmetric-definite generalized eigenproblem whose eigenvalues are lowest. The filter we use is a Chebyshev polynomial composed of a linear combination of a small number of resolvents and an identity. In present study, all shifts of the resolvents used are restricted to real numbers less than the lowest eigenvalue. Then the filter's transmission function is a Chebyshev polynomial composed of a rational function of the eigenvalue. And the rational function is a sum of a small number of the inverses of the shifted eigenvalues and a constant.

For each case of the number of resolvents is from one to three, for the specified three important parameters on the shape of the filter's transmission function, we try to find the combination of the degree of the Chebyshev polynomial and the rational function. If it exists, correspondingly the filter can be constructed as the Chebyshev polynomial of the linear combination of resolvents and an identity. To find the combination, first the degree of the Chebyshev polynomial is assumed, and then the shifts and the constant which determine the rational function are searched, so that the ranges of the value of the rational function satisfy conditions in three regions of eigenvalue of the filter namely the pass-band, the transition-band and the stop-band. When complex shifts were allowed, for any number of resolvents the rational function was given from the best approximation theory. But the theory does not apply when shifts are restricted to be real, and the filter's transmission properties become not very good.

By restricting shifts to real, we have an advantage especially when the system of linear equations is solved by some matrix factorization method. The computational requirement of an application of a resolvent by solving a system of linear equations is reduced when the shift is real than it is imaginary. For example, the amount of storage required with real shift is about a half of that with imaginary shift. The count of arithmetic operation is also reduced. But, the poor properties of filter's transmission when all shifts are reals may require the repeated applications of the filter or increased number of vectors to be filtered than when shifts are complex numbers especially when higher accuracies of eigenpairs are desired.

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First order least-squares formulations for eigenvalue problems

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Key Words: *First order least-squares, eigenvalue problems*

In this talk we discuss spectral properties of operators associated with the least-squares finite element approximation of elliptic partial differential equations. The convergence of the discrete eigenvalues and eigenfunctions towards the corresponding continuous eigenmodes is studied and analyzed. a priori and a posteriori estimates are proved in the Poisson and linear elastic case.

Applications to vibration analysis in elastic structures and in problems concerning the fluid–structure interactions are presented. In fact, the common way to determine vibration modes, the primal approach based on the minimization of an energy depending on the displacement variable does not lead to uniform accuracy for nearly incompressible materials such as common blood vessel walls or the heart muscle, except if the degree of the polynomial approximation is kept very high, leading to a high computational effort.

Stresses can be computed from the primal approach in post-processing, but this approach leads to stresses where divergence is not squarely integrable. They are not H(div)-conforming and surface or interface traction forces cannot be evaluated. Moreover, momentum cannot be conserved exactly. As these quantities are driving quantities, the standard methods are not accurate enough in many challenging applications and stress-based methods are known to be a game changer. However, the symmetric gradient arising in the corresponding PDE is a difficult condition to impose at the discrete level. The conforming discretization of those stresses (so-called Arnold-Winther approach [1]) is sophisticated and increases the computational cost enormously. To develop a new class of extremely efficient numerical methods that compute vibrations with high guaranteed accuracy,

One of the major advantages of the Least-Squares method, is the symmetry and positive definiteness of the formulation. At first glance, the consideration for eigenvalue problems seems to conserve neither the minimization property nor the symmetry and complex approximations were obtained in [2]. However, [3] shows that the symmetry of the methods can be recovered, as well as the inherent error estimator. The approach leads to optimal convergence of the eigenvalues.

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Matrix-Less Eigensolver for Large Structured Matrices

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Key Words: Structured Matrices, Discretization Matrices, Generalized Locally Toeplitz Sequences, Eigenvalues, Eigenvalue Expansion, Eigensolver, Interpolation and Extrapolation

Sequences of structured matrices of increasing size arise in many scientific applications and especially in the numerical discretization of linear differential problems. We assume as a working hypothesis that the eigenvalues of a matrix X_n belonging to a sequence of this kind are given by a regular expansion. Based on this working hypothesis, which is illustrated to be plausible through numerical experiments, we propose an eigensolver [1] for the computation of the eigenvalues of X_n for large n. The eigensolver is called matrix-less because it does not operate on the matrix X_n but on a few similar matrices of smaller size combined with an interpolation-extrapolation strategy. Its performance is benchmarked on several numerical examples, with a special focus on matrices arising from the discretization of differential problems, and turns out to be quite satisfactory in all cases.

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On the Matrices in B-spline Collocation Methods for Riesz Fractional Equations and their Spectral Properties

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Key Words: Fractional Operators, B-spline Collocation, Toeplitz Matrices, Spectral Analysis

Fractional operators, see e.g. [3], are a mathematical tool that received much attention in the last decades because of their non-local behavior which has been demonstrated to be useful when modeling anomalous diffusion phenomena appearing, e.g., in imaging or electrophysiology. The improved physical description of the considered phenomenon obtained by replacing a standard derivative with a fractional one, however, translates in a more challenging numerical treatment of the corresponding discretized problems. Indeed, even when standard local discretization methods are adopted, the non-locality of the fractional operators causes absence of sparsity in the discretization matrices. This makes fractional problems computationally more demanding than standard partial differential problems and stresses the need of a proper numerical linear algebra analysis.

In this work, we focus on a fractional differential equation of order α in Riesz form discretized by a polynomial B-spline collocation method [2]. For an arbitrary polynomial degree p, we show that the resulting coefficient matrices possess a Toeplitz-like structure [1]. As such, we investigate their spectral properties via their symbol, a function which describes the asymptotic spectral distribution of a sequence of matrices, as the size tends to infinity. We prove that, like for second order differential problems, also in this case the given matrices are ill-conditioned both in the low and high frequencies for large p, with a mitigated conditioning in the low frequencies and a deterioration in the high ones. Moreover, as a side result of the symbol computation, we are able to express the central entries of the coefficient matrix as inner products of two fractional derivatives of cardinal B-splines. Finally, we perform a numerical study of the approximation behavior of polynomial B-spline collocation which suggests that the approximation order for smooth solutions is $p+2-\alpha$ for even p, and $p+1-\alpha$ for odd p.

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Optimization Methods for One Dimensional Elastodynamics

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Key Words: Elastodynamics, Optimization, Galerkin methods

In [1] the system of elastodynamics in 1D was discretised in time and the resulting semidiscrete scheme is shown to admit a variational formulation. The solutions of this variational problem are shown to converge as the discretization parameter vanishes, in some sense, to the solution of the original continuous problem. This approach can be extended also to higher dimensions and produces solutions which are admissible in the sense that satisfy entropy inequalities. In this work we consider this approach from the point of view of constructing a new class of numerical schemes for approximating solutions to the system of elastodynamics. The approximation is associated to viewing the equations of elasticity as a Hamiltonian system, and considering the time-discretization of the dynamics.

The basic idea of the time discrete scheme is that given the solution at the first $j-1$ time steps, j-th time step is approximated by solving a constrained minimization problem. We propose a fully discrete scheme where we minimize the associated functional using optimization techniques. The fully discrete scheme is based on the continuous or discontinuous Galerkin finite element method, [2, 3]. The Gradient Descent method is utillized for approximating solutions to the optimization problem and it's enhanced with various accelerating techniques for overcoming well known pitfalls of the algorithm.

We investigate the computational efficiency and stability of the new class of schemes and we compare them with the standard finite volume and discontinuous Galerkin schemes for conservation laws. We consider test cases with smooth and non-smooth solutions and the preliminary results are very encouraging.

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Refined Isogeometric Analysis for Quadratic Eigensystems of Vector-valued Multifield Problems

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Key Words: Quadratic eigenproblems, Refined isogeometric analysis, Krylov eigensolvers.

We propose to use refined isogeometric analysis (rIGA) [1] to solve quadratic eigenproblems. rIGA, while conserving desirable properties of maximum-continuity isogeometric analysis (IGA), reduces the interconnection between degrees of freedom by adding low-continuity basis functions. Herein, we consider rIGA and IGA discretizations when employing Krylov eigensolvers to solve quadratic eigensystems arising in 2D vector-valued multifield problems. We use C^0 and C^1 separators at certain element interfaces for our rIGA generalizations of the curl-conforming Nédélec and divergence-conforming Raviart–Thomas finite elements [2]. For large problem sizes, the eigencomputation cost is governed by the cost of LU factorization [3], followed by costs of matrix–vector and vector–vector multiplications in the sense of Krylov projection. Let p be the polynomial degree of basis functions, the LU factorization is up to $\mathcal{O}\big((p-1)^2\big)$ times faster when using rIGA compared to IGA in the asymptotic regime. Thus, rIGA theoretically improves the total eigencomputation cost by $\mathcal{O}\big((p-1)^2\big)$ for sufficiently large problem sizes. In practical moderate-size problems, the improvement rate deteriorates when increasing the number of requested eigenvalues because of multiple matrix–vector and vector–vector operations. Our numerical tests show rIGA improves the total eigencomputation cost of quadratic eigensystems by $\mathcal{O}(p-1)$ for moderately sized problems when we seek to compute a reasonable number of eigenvalues.

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SoftFEM/SoftIGA for Eigenvalue Problems

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Key Words: eigenvalue, elliptic operator, finite element method, isogeometric analysis

I this talk, the speaker will present the recently developed methods, namely, the soft finite element method (softFEM) and the soft isogeometric analysis (softIGA), for solving the elliptic eigenvalue problem. The prefix "soft" refers to the main idea that the stiffness of the discretized system is softened. We remove the non-physical energy associated with the high-frequencies in the spectrum via penalty terms with negative coefficients . At the matrix level, this means that condition number is reduced. The stiffness (or condition number) reduction ratio scales linearly with the oder of the underlying element and is $1 + \frac{p}{2}$ for softFEM (FEM to softFEM raito). The two key advantages are to improve the approximation of the eigenvalues in the upper part of the discrete spectrum and to reduce the condition number of the stiffness matrix. In the end, the speaker will discuss how these methods can be applied to time-dependent problems with larger time steps for explicit time-marching schemes while ensuring the stability.

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VEM Discretization of PDE Eigenvalue Problems: Effect of the Stabilization Parameters

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Key Words: Partial differential equation, eigenvalue problem, virtual element method, parameter dependent matrices

In this talk we consider the virtual element approximation of the solution of eigenvalue problems associated with partial differential equations. Due to the need of stabilizing the bilinear forms involved in the discrete formulation of the problem, the matrices appearing in the associated generalized eigenvalue system might depend on parameters (see [1]). We discuss how the presence of such parameters can produce unexpected results even in the approximation of the Laplace eigenvalue problem and try to address the question of finding the best choice in order to achieve spectral correctness together with optimal approximation properties. The virtual element approximation of eigenvalue problems for several applications has been investigated in recent years, however the question of the choice of the optimal parameters is only occasionally addressed (see [2] for a survey). We investigate further the VEM discretization of the acoustic vibration problem, and show that in this case there is no need of using any stabilization for the stiffness and mass matrix.

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A new variant of AINV preconditioning simplified by using nonzero element positions of a coefficient matrix

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Key Words: approximate inverse preconditioning, Krylov subspace method, graphics processing unit

In recent years, graphics processing units (GPUs) have been used to efficiently solve a linear system by means of a preconditioned Krylov subspace iterative method. To fully exploit the potential of GPUs for massive data processing, the preconditioner is required to have a high degree of parallelism. Whereas most ILU–type preconditioners, based on the ILU (or IC) factorization, require forward/backward substitution in their preconditioning operations, the approximate inverse (AINV) preconditioner [1], which is one of the sparse approximate inverse preconditioners, is implemented by sparse matrix-vector multiplication (SpMV). SpMV has a higher degree of parallelism than the forward/backward substitution because SpMV does not involve data dependencies, unlike the forward/backward substitution. From this perspective, the AINV preconditioner is more suitable for execution on GPUs than the ILU–type preconditioners. However, the incomplete conjugate algorithm (AINV algorithm), which constructs the AINV preconditioner, tends to take a long time compared to the ILU factorization [2]. Therefore, it is important to improve the AINV algorithm to make AINV preconditioning more attractive.

Considering this background, we propose a new version of the AINV algorithm: position-based simplified AINV (PS-AINV) algorithm. The basic idea of the PS-AINV algorithm is to simplify the standard AINV algorithm based on the positions of the nonzero elements of a coefficient matrix. Thanks to the simplification, the PS-AINV algorithm not only runs faster but also has coarse-grained parallelism; that is, speed-ups by both simplification itself and multi-thread parallelization are expected. Numerical results showed that the PS-AINV algorithm constructs the preconditioner faster than the standard AINV algorithm without significant performance degradation in the iterative part. As a result, the performance of the whole solver (the sum of preconditioner construction and PCG iteration) was also improved.

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Auto-tuning for Computation Accuracy and Power Consumption by ppOpen-AT

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Key Words: *Mixed Precision, Energy Optimization, Auto-tuning, ppOpen-AT*

To have a technological breakthrough in Post Moore's era, several challenges have been studied. One of promising approaches is utilizing mixed precision computations to obtain speedup and low power computations. However, it is not easy way to adapt mixed precision computations to arbitrary codes, since the speedup factors depends on hardware. In addition, down of computation accuracy also depends on nature of treated numerical problems.

To shove the above problem, we propose an auto-tuning (AT) function for dedicated AT language, named ppOpen-AT [1]. The ppOpen-AT is a directive-based computer language to adapt AT function into arbitrary parts of programs. The proposed function can specify lower types of accuracies into the following two parts: (1) Specified variables or arrays (SVA) in definition parts in program; (2) Specified blocks in the program (SBP).

To autotune its computational accuracy, software developers need to specify acceptable down of accuracies in advance for software developers. After specified targets of changing accuracies, code generator of ppOpen-AT generates all combinations of candidate codes. There is an additional process is automatically generated in the target parts, such as copies and stores from arrays with higher precision to arrays with lower precision. This causes overhead of execution time, and additional power consumptions for the generated code.

Effectiveness of the proposed functions are evaluated with NICAM [2], which is a practical numerical simulation code with global cloud resolving model. In this evaluation, we use a part of tiny cloud physical computations. The part consist of a subroutine of **physicskernel_microphysics** in **mod_mp_nsw6.f90** in NICAM benchmark, **nicam_dckernel_2016**. Target part is a three-folded loop with heavy loop body for computations. In this evaluation, length of loop is fixed. There are several output values after exiting the target loop. Hence computations with lower accuracies directly affect computational accuracies.

Result of the above evaluation indicates that: (1) speedup factor of 1.04x and 1.06x reduction of energy consumption by keeping accuracy of 1.E-13 for the SVA; (2) speedup factor of 1.12x and 1.06x reduction of energy consumption, if we accept down of accuracy for 3.E-4 for the SBP.

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Challenges of Heterogeneous Coupling

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Key Words: *Heterogeneous system, Coupled simulation, Atmospheric model, Machine learning*

In this presentation, we discuss coupled computation of multiple models in a heterogeneous system consisting of a group of nodes with different architectures. This computation is referred to as heterogeneous coupling, and we introduce our studies on heterogeneous coupling.
The system utilized herein is the Wisteria/BDEC-01 of the University of Tokyo. Wisteria/BDEC-01 is a hybrid system with two groups of compute nodes: simulation nodes (Odyssey), which equips A64FX, and data/learning nodes (Aquarius) with Intel Xeon processors and NVIDIA A100 Tensor Core GPUs. Additionally, the target programs are the atmospheric model, NICAM [1], and the data analysis software, ADA. Herein, ADA is applied to the machine learning library PyTorch. This study aims to couple NICAM on Odyssey and ADA on Aquarius, as well as perform real-time machine learning on the computed values of NICAM.
To achieve this goal, we developed two software packages; WaitIO-Socket, which is a low-level data communication software, and h3-Open-UTIL/MP [2], which is a general-purpose coupling software. In general, MPI is used for data communication between programs in MPMD calculation. However, MPI library cannot be applied between Odyssey and Aquarius. Therefore, we developed the WaitIO-Socket to realize the communication between the two systems.
It uses TCP/IP for communication and implements an MPI-compliant interface. h3-Open-UTIL/MP is a coupling software that performs grid remapping and data exchange among multiple models. For NICAM-ADA coupling, h3-Open-UTIL/MP is utilized to convert NICAM data of high-resolution grid to low-resolution grid for machine learning. Originally, only MPI communication was implemented in the h3-Open-UTIL/MP, and heterogeneous coupling between Odyssey and Aquarius becomes possible by adding WaitIO-Socket.
The problem with heterogeneous coupling is the computation speed when using processors of different architectures and the communication speed between different machines. NICAM has been tuned to provide sufficient calculation performance on the Odyssey's A64FX. Conversely, PyTorch, as it is called by ADA, supports GPUs and can perform fast operations on Aquarius' Tensor Core. Therefore, both models are well suited for their respective machine architectures based on computational speed. For the communication speed, a test program with the same number of grid points as that of the NICAM-ADA coupling confirmed that practical performance could be obtained.

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h3-Open-BDEC: Innovative Software Infrastructure for Scientific Computing in the Exascale Era by Integrations of (Simulation + Data + Learning)

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Key Words: *Computing by Adaptive Precision, Machine Learning, Data Analytics*

We are developing an innovative method for computational science for sustainable promotion of scientific discovery by supercomputers in the Exascale Era by combining (Simulation + Data + Learning (S+D+L)). The Wisteria/BDEC-01 system (Big Data & Extreme Computing), which started its operation in May 2021 at the Information Technology Center, the Tokyo University, is a Hierarchical, Hybrid, Heterogeneous (h3) system, which consists of computing nodes for computational science and engineering with A64FX (simulation nodes) and those for data analytics/AI with NVIDIA A100 GPU's (data/learning nodes).

In this study, we consider the Wisteria/BDEC-01 as the platform for integration of (S+D+L), develop an innovative software infrastructure "h3-Open-BDEC" for integration of (S+D+L), and evaluate the effects of integration of (S+D+L) on the Wisteria/BDEC-01 system. The h3-Open-BDEC is designed for extracting the maximum performance of the supercomputers with minimum energy consumption focusing on (1) innovative method for numerical analysis with high-performance/high-reliability/power-saving based on the new principle of computing by adaptive precision, accuracy verification and automatic tuning, and (2) Hierarchical Data Driven Approach (hDDA) based on machine learning.

The h3-Open-BDEC is the first innovative software platform to realize integration of (S+D+L) on supercomputers in the Exascale Era, where computational scientists can achieve such integration without supports by other experts. Source codes and documents are open to public for various kinds of computational environments. This integration by h3-Open-BDEC enables significant reduction of computations and power consumptions, compared to those by conventional simulations.

This talk overviews the h3-Open-BDEC project, summarizes the various achievements and results, and provides future perspective. of the recent progress

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Improved Initial Approximations for Pressure Correction Schemes

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Key Words: *Multigrid, Incompressible Flow, Computational Fluid Dynamics, Pressure Correction, Conjugate Gradient Method, Parallel Computing, Large Scale Systems, Navier Stokes*

Numerical simulations for the incompressible Navier-Stokes equations are most often solved using a pressure correction scheme, such as Marker-and-Cell type methods, or the SIMPLE method. These methods bind the continuity equation to the pressure in order to solve the non-linear momentum and velocity terms implicitly. These semi-implicit methods lead to a pressure correction scheme in the form of a discretized Poisson equation. Despite pressure being generally undesired in applications, solving the system equations derived from the Poisson equation takes the majority of computational cost in these types of methods.

These large scale systems are generally solved using a preconditioned iterative method, such as the conjugate gradient method. While traditionally, the CG method begins with a 0 vector initial estimate, we use information from previous time steps, previous pressure correction equations, information about the system, and information about the preconditioned iterative method itself to predict an initial approximation vector that can be used to improve convergence of the iterative method, thus decreasing overall computation time.

In particular, we use a machine learning scheme to predict the right hand side of the system of equations, allowing us to solve an approximate problem in parallel, in advance. The solution to this approximate problem is used as an initial estimate for the true problem when it is derived by one of the semi-implicit methods above. This leads to a faster algorithm overall.

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15th World Congress on Computational Mechanics (WCCM-XV)
8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII)
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Performance improvement of immersed boundary-lattice Boltzmann method on multiple GPUs

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Key Words: Immersed boundary method, Lattice Boltzmann method, High performance computing, GPU acceleration

Computational fluid dynamics (CFD) are recently used in a broad field, such as industrial, medical and video. In CFD, the simulation of flow around objects moving freely is called as moving boundary flow, and it is one of important themes of CFD. In order to solve moving boundary flow quickly, we use immersed boundary-lattice Boltzmann method (IB-LBM), which is easy to parallel computing using GPU. The parallel computing shortens the computing time of IB-LBM, and using multiple GPUs does more. However, in multi-GPU computing, it is necessary to communicate data between GPUs. It results in decrease of parallel efficiency.

We implement IB-LBM in three ways in order to increase parallel efficiency. One implementation is naive. In another implementation, we reduce amount of communication data, for example, considering the velocity direction of particles. In the other implementation, calculation time hides communication time. CPU communicates data while GPU computes domain that is not related to communication. As a result, second implementation improve performance of IB-LBM, and third more.

In addition, we evaluate performance of IB-LBM, changing the way to assign GPUs to subdomains when two dimension split. Split direction and whether GPUs are in same compute node affect communication time between the GPUs. In order to hide communication time to the fullest extent, we have to assign GPUs to subdomains properly. By doing this, we improve performance of IB-LBM.

In this talk, we present the implementation of IB-LBM and assigning GPUs to subdomains properly, and show the performance improvement by the implementation and the way to assign GPUs.

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Performance Optimization Of Lattice Boltzmann Method On A64FX

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Key Words: A64FX, Lattice Boltzmann method, optimization

A64FX is processor made by Fujitsu. It is famous for Fugaku which is the fastest supercomputer in the world at TOP500 which is performance ranking of the Linpack benchmark. The feature of A64FX is 64-bit ARM architecture and Scalable Vector Extension SIMD instruction. Moreover, one A64FX chip is consist of 4 Core Memory Group (CMG) that has 13 cores (12 calculation core and 1 assistant core), 2nd cache, and memory controller. As a result of it, we have to consider it when you do optimization of software. The performance of system which installs A64FX in TOP500 is very good, although we have to think about general purpose of using A64FX. And to do it, we must know the characteristics of processor and compiler. The object of this talk is it.

In HPC field, computational fluid dynamics (CFD) is one of the popular research subjects because of its amount of calculation. Lattice Boltzmann methods (LBM) is popular and often used because we can provide better performance easily with parallel computing. It is consist of streaming process and collision process. Streaming process is memory copy part. Collision process is calculation part. Therefore, performance of LBM is an important optimization problem and a good benchmark of supercomputer.

As a part of this study, we first optimize LBM with 1 CMG on A64FX at Wisteria-Odyssey that is operated at Information Technology Center, The University of Tokyo. We use (x, y, z) = (256, 256, 256) grid point simulation and D3Q27 model. The baseline optimization is very important. For example, blocking algorithm and code style for compiler SIMD optimization are effective. Secondly, we work on the optimization of 1 core (4 CMGs). We have to consider the communication between CMGs. Lastly, we optimize LBM with many cores.

In this talk, we provide the optimization method of LBM on A64FX, and difficulty information. We also show the result of optimization of LBM. For example, blocking and compiler SIMD optimization are very important.

A Novel Method to Impose Velocity Boundary Conditions for Eulerian Fluid-structure Interaction Scheme Using Lagrangian Marker Particles

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Key Words: *Fluid-Structure Interaction, Eulerian Formulation, Immersed Boundary Method, Particle Method*

A full Eulerian fluid-structure interaction (FSI) formulation is an attractive method for high-performance computing and treating large deformation of solid. In this method, motions of solid and fluid are numerically solved with a spatially fixed mesh. In short, material interfaces cannot be captured by computational meshes and need to be represented by a color function in this method. Conventional full Eulerian methods cannot avoid the numerical dissipation of interfaces due to solving their advection equations. And also, imposing velocity boundary conditions to arbitrary positions and shapes in a computational domain.

In order to overcome the numerical dissipation of interfaces, we have proposed the full Eulerian FSI formulation with Lagrangian marker particles[1]. However, it is still difficult to impose velocity boundary conditions for arbitrary positions and shapes in a computational domain. For non-conforming mesh methods, immersed boundary methods have been proposed to impose velocity boundary conditions to arbitrary positions and shapes. Thus, in this research, we introduce the immersed boundary method[2] to our method[1] to impose velocity boundary conditions for arbitrary positions and shapes in a computational domain.

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A Study of Phase-Field Parameters in Gas-Liquid Two-Phase Flow Problems

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Key Words: *Computational fluid dynamics, Two-phase flow, Phase field*

ABSTRACT

A multi-phase multi-component thermal-hydraulic simulation code JUPITER[1] has been developed to analyze the molten material behaviour under severe accident conditions in nuclear reactors. In JUPITER, the THINC/WLIC method[2] was implemented as an interface tracking method, which enabled us to accurately calculate the dynamics of the multiphase interface of the molten material at relatively low flow velocity. However, when JUPITER is applied to air-water two phase flows in fuel bundles, there is a problem that the Volume of Fluid (VOF) value is stripped from the interface and small VOF values drift in turbulent flows where coalescence and separation of the interface are active. To improve the interface tracking method of the JUPITER code, the applicability of the phase-field method[3] has been investigated. In this study, the phase-field method is applied to the JUPITER code and the droplet oscillation phenomena are analyzed. The numerical results are compared with the theoretical solution to clarify the sensitivity of the phase-field method to its hyperparameters such as the mobility and the interface width.

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A Weakly Compressible Flow Computation of Liquid Film with Interface-adapted AMR method

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Key Words: *Liquid film, Surfactant, Langmuir model, Tree-based AMR method, GPU computing*

Direct numerical simulation of the formation and rupture of thin liquid film is performed by using weakly compressible scheme with interface-adapted adaptive mesh refinement (AMR) method. In conventional semi-implicit method that solves the pressure Poisson equation to solve the incompressible two-phase flows, the computational cost increases drastically as the size of problem becomes larger, which cause a severe scalability problem and is not suitable for parallel computing. Based on low-Mach-number assumption and isothermal Navier-Stokes equation, an independent hyperbolic pressure evolution equation is derived and a fully explicit time integration that has good scalability and efficiency is developed.

To capture the moving gas-liquid interface, a coupled phase-field and level-set method is developed. Finite Volume Method (FVM) is used to solve the conservative Allen-Cahn equation and conserve the total mass of each phase. The normal vector of interface used in Allen-Cahn is derived by level-set function, which can provide better accuracy. The time evolution of level-set function is based on advection. Level-set function is re-initialized by phase-field function every several dozen steps during the simulation to keep the unique property that the absolute value of the gradient of level-set function is one.

GPU code for parallel computing based on CUDA is developed for a tree-based AMR that is able to reduce the computational cost by assigning a high-resolution mesh around the moving interface region automatically. A two-dimensional soap bubble growing simulation is performed with and without considering the Marangoni effect caused by the transportation of surfactant. Langmuir model is adopted to numerically describe the adsorption and desorption of surfactant on the liquid-gas interface. The finest cell size is 0.0195mm, which is equivalent to 8,192×8,192 uniform cells. This computation indicates that the behavior of the thin liquid film is reproduced by the explicit scheme and AMR method.

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Acceleration of Phase-field Data Assimilation using Multiple-GPU Parallel Computing to Infer Interfacial Properties of Zinc Alloys

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Key Words: *Hot-dip Galvanizing, Dendrite, Solidification, Phase-field Method, Data Assimilation, High-performance Computing*

Hot-dip galvanizing (HDG) is a surface coating technology used for corrosion protection of steel; it is widely used for commercial purposes because by employing this method, steel can be mass-produced using continuous HDG lines. Surfaces of HDG films have a shiny and beautiful texture, termed as “spangle,” which greatly influences corrosion resistance and appearance. Therefore, it is essential to reveal the formation mechanism of the spangle texture during galvanization.

Recently, Takaki et al. [1] and Kim et al. [2] conducted phase-field simulations to reveal the formation mechanism of the spangle texture, and both the studies revealed that the characteristic interfacial properties lead to the formation of this texture. However, very little information regarding the true interfacial properties of zinc alloys is available. Data assimilation is a promising method for inferring material properties; this method combines experimental observations and numerical simulations [3]. However, it incurs large computational costs, as multiple numerical simulations with different material properties and/or computational conditions are involved.

In this study, we accelerated data assimilation for three-dimensional dendrite growth simulations using the phase-field method by employing parallel computing schemes using multiple graphics processing units. We used an efficient data assimilation technique, that is, the local ensemble Karman filter. The accuracy of the assimilation was confirmed via twin experiments. In the near future, we aim to combine time-resolved X-ray tomography [4] and large-scale phase-field simulation to infer the interfacial properties of zinc alloys, which are used as HDG materials.

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Combining Phase-field and VOF Methods with a Conservative Weakly Compressible Solver for Large-scale Two-phase Flow Simulation

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Key Words: *Weakly Compressible, Consistent Transport, Two-phase Flow, Multi-GPU*

In recent years, the use of GPU as computational accelerator has attracted wide attention. Powerful computing performance and high bandwidth for data transfer are the main features of GPU. In the simulation of incompressible fluid flow, a Poisson equation should be solved implicitly. This poses a great challenge for massively parallel and scalable computing because of the complexity in the iteration algorithms and the slow convergence rate for two-phase flows with a high density contrast. On the other hand, weakly compressible Navier-Stokes equations are becoming a popular alternative for simulation of incompressible fluid flows. A pressure evolution equation can be derived under the low Mach number and isothermal condition. Recently, a weakly compressible scheme with adaptive mesh refinement has been successfully applied to simulate two-phase flows [1].

To address the demand for high-performance large-scale simulation of two-phase flows, a momentum-conserving weakly compressible Navier-Stokes solver with multi-GPU computation is proposed. Following the principle of consistent transport, the Con-CAC-LS solver that involves conservative Allen-Cahn equation and level-set method and the Con-PLIC-HF solver that involves PLIC-VOF and height function method are developed. Combined with the evolving pressure projection method to damp the acoustic wave [2], this solver aims at a robust and accurate computation of violent two-phase flows with a high density ratio, while taking advantage of fully explicit time integration of the weakly compressible Navier-Stokes equations.

For multi-GPU computation, the strong scaling with two types of domain partition is evaluated and a better scalability is exhibited by the 3D partition. The technique for overlapping communication and computation is implemented and discussed. Finally, the conservative solvers are used to simulate the Rayleigh-Taylor instability, milk crown, dam break and liquid jet atomization problems. Accurate and delicate evolution process of the two-phase interface is demonstrated.

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Efficient parallel mesh movement based on fast low rank solvers and local remeshing

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We propose in this work a framework dedicated to the movement of rigid bodies inside 3 dimensional complex geometries which are discretized with conformal unstructured meshes. Several applications can take benefit from this framework such as shape design and Fluid Structure Interactions (FSI) to name a few. This paper will focus on FSI applications. The displacement imposed on the rigid bodies is smoothly interpolated to the mesh elements inside the domain to deform the whole mesh with respect to the prescribed displacement. The mesh movement is considered to be part of mesh deformation problems. In this work, Radial Basis Functions (RBF) interpolation method is used to deform the mesh. This algebraic interpolation approach is well known for its robustness, but it is too expensive on large scale meshes.

The objectives of this work are twofold: 1- Speeding up the RBF calculations in a large-scale parallel environment. Indeed, the resulting linear system has a good hierarchical matrix structure which is exploited to build a parallel hierarchical low-rank solver to speed up the mesh deformation interpolation. The low-rank approximation is driven by a predefined error tolerance. 2- Combine the RBF computed displacement with local remeshing to prevent mesh invalidity during long term displacements or large deformation. The displacement field is used to predict bad quality elements to be locally remeshed. A metric based on the displacement field is derived to inform the remeshing tool which element is subject to local modification. The remeshing is performed in parallel as well the whole the computation pipeline.

Numerical experiments were conducted on numerous 2D and 3D complex geometries with deep analysis on convergence, mesh quality and performance. The results and performance assessments will be presented.

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Eulerian Elastoplastic Analysis Using Lagrangian Particles for Resin Material

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Key Words: Cartesian Mesh, Eulerian Method, Resin Material,

Resin parts have been widely used as load-carrying components in many mechanical engineering fields. Thus, engineers must deeply consider estimating the mechanical material property and understanding the mechanical response. In many cases, the finite element method (FEM) is employed to predict the mechanical property and response. It is necessary to divide the target component into the mesh for FEM. However, the complicated component and/or whole structure is difficult to divide the mesh, furthermore, high computational cost.

In this study, we propose a structural simulation based on the Eulerian formulation using marker particles [1] for resin materials. The proposed method represents the target components by particles in a fixed Cartesian mesh. As a result, it is possible to avoid the numerical diffusion of the solid interface and the solid internal variables. Furthermore, it is suitable for high-performance computing. The conventional method is applied to the elastic or elastoplastic material under large deformation. Considering this, implementing the material model for resin material[2] based on the elastoplastic formulation.

We demonstrate representative numerical examples to evaluate the validity of the present method. The numerical result is compared with the FEM and/or experimental results from the point of view of the deformed shape and stress value.

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Flow Field Data Mining of Automobile Models with Pareto-Optimal Aerodynamic Shape Using Proper Orthogonal Decomposition

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Key Words: *Proper Orthogonal Decomposition, Flow Structure, Automobile Aerodynamics*

There are multi objectives in the aerodynamic development of automobiles, which are not only drag reduction but also improvement of running stability, aeroacoustic noise reduction, thermal cooling, etc.. In recent years, with the development of high-performance computing technology, a computational fluid dynamics (CFD)-based multi-objective shape optimization for automobile aerodynamics is being realized. To contribute to actual product development and support design engineers, it is also important to extract useful knowledge for design from the Pareto solutions of the multi-objective optimization. The proper orthogonal decomposition (POD) is a powerful technique for such data mining from the Pareto solutions [1, 2]. Automobile aerodynamics engineers has conventionally discussed the relationship between aerodynamic performance and flow phenomenon focusing on the flow structure and topology around automobile.
Therefore, in this study, we applied the POD to extract characteristic flow structures as the POD modes of time-averaged velocity field from the results of aerodynamic shape optimization for a 1/5 scale sedan-type automobile model [3]. Relationship between extracted flow structures and aerodynamic performances of the automobile model was statistically analysed and the flow phenomena related to the Paleto-optimal aerodynamic characteristics were clarified.
The aerodynamics analysis for each sample of the evolutionary multi-objective optimization had been conducted by using the building cube method (BCM) with the immersed boundary method (IBM). The time-averaged velocity field in approximately 200 samples, analysed during the optimization, were analysed by the POD. As the principal component regression (PCR), regression analysis between the mode coefficients and the objective functions was performed, and the POD modes related to the objective aerodynamic performances were investigated.

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Implementation of the Mother-leaf Method on GPU-accelerated AMR Code for Phase-field Computation of Dendrite Growth

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Key Words: *Phase-field Method, Adaptive Mesh Refinement Method, Mother-leaf Method, GPU Computation, Solidification*

The phase-field (PF) method is the only numerical method that can quantitatively predict dendrite growth. However, it has the disadvantage of a high computational cost because it is based on a diffuse interface model. To accelerate the PF computations, parallel computations have been conducted using multiple graphic processing units (GPUs), which exhibit high parallel processing performance. Alternatively, the adaptive mesh refinement (AMR) method, in which fine meshes are arranged only around the interface, has also been used to improve computational efficiency.

Through the combined use of parallel GPUs and AMR, further acceleration of PF computations for dendrite growth has been achieved [1]. However, because of the use of AMR, the execution time of PF computation for each grid point increases several times as compared to that with a uniform mesh. In the previous study, a block-structured AMR method was used, which offers the advantage of sequential memory access when computing the PF model using a finite difference method [1]. However, the method requires memory access for reading grid-point data on adjacent blocks to compute the outer grid points of the blocks. This process generates multiple branch divergence depending on the position of the outer grid points and the difference level from the adjacent blocks, which degrades the execution rate of the GPU.

In the present study, to solve the degradation of computational speed in the previous reports [1], the mother-leaf method [2] has been implemented on the parallel GPUs code with AMR of a PF dendrite growth simulation. The mother-leaf method reduces the total number of outer grid points of blocks by allocating each block to the parent node of leaf nodes. The computational performance of the developed method has been compared with the results of previous studies [1] to evaluate the improvements in computational efficiency.

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Large-scale Simulation for a Real Driftwood Disaster by Using LBM with AMR

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Key Words: *CFD, Cumulant LBM, DEM, HPC, CUDA, AMR*

The flood poses a great threat to the safety of human lives and properties, when it accompanies floating objects such as driftwood, damage is multiplied [1]. In this study, computational fluid dynamics (CFD) based simulations for the motion and mechanical properties of driftwood are carried out. The cumulant lattice Boltzmann method (LBM) [2] and discrete element method (DEM) are utilized to simulate fluid phase and solid phase respectively. For the interface capturing method, a conservative Allen-Cahn equation is employed to maintain the mass conservation. In order to achieve high performance computing (HPC), CUDA programming and adaptive mesh refinement (AMR) [3] method are applied.

The driftwood capturing experiments in water tank were simulated first for validation. By comparing the snapshots, water height and force, it can be concluded our simulation results show good agreement with experimental results, proving that our method is appropriate for driftwood simulation.

After the validation process, simulations of the actual driftwood disaster happened in Otomo area of Iwate Prefecture were performed. By using AMR method, the number of meshes is reduced by around 78% compared to using uniform meshes. Results showed that accumulation positions of driftwood in simulation have a good agreement with that of real situation.

In conclusion, large-scale simulations of driftwood disasters using GPU supercomputers show that the simulation results exhibit a certain degree of agreement with the actual situations. The simulation method is of great significance for driftwood disaster prediction and prevention.

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Lattice Boltzmann Simulation with Actuator Line Model for Tidal Current Turbines on Multiple GPUs

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Key Words: *Tidal current turbines, Lattice Boltzmann method, Actuator line model, GPU*

In numerical simulations of tidal current power generation farms, large-scale CFD simulations with a high-resolution grid are required to calculate the interactions between tidal turbine wakes. In this study, we develop a numerical simulation method for tidal current turbines using the lattice Boltzmann method (LBM), which is suitable for large-scale CFD simulations. Turbines are modeled using the actuator line model (ACL)[1], which represents each blade as a point cloud. In order to validate our LBM-ACL model, we conducted a water tank experiment with two turbines and simulated the same conditions as in the experiment. The time series of the calculated and experimentally measured torques oscillate regularly, which is the effect of the regular waves. The torque of the backward turbine is smaller than that of the upstream turbine, which is due to the velocity deficit of the wake of the upstream turbine. LBM simulations could reproduce the experiment in terms of wake interaction and wave effects on turbine performance, and we confirmed the validity of the LBM-ACL approach. Our LBM-ACL code can be applied for a tidal current power farm, and we demonstrated a simulation for ten tidal current power farm with 80 turbines using 1.48 billion grid points and 16 GPUs Tesla P100 on the multi-GPU system ITO subsystem B at Kyushu University.

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Real-World Aerodynamics Assessment for Road Vehicle Development Realized on the Supercomputer "Fugaku"

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Key Words: *CFD, Real-World, Road Vehicle, Supercomputer, Fugaku*

Conventional assessment of vehicle aerodynamic performance has been conducted under uniform flow conditions using both experiments in wind tunnels and simulations. However, unsteady aerodynamic forces always act on a road vehicle in the practical environment due to atmospheric turbulence and vehicle motion, which affect the vehicle's steering and fuel consumption. Therefore, there is a need for a method to predict such unsteady aerodynamic forces with high accuracy and to assess the aerodynamic performance of vehicles under practical driving conditions.

In this study, we developed a coupled analysis framework using CUBE, a fluid analysis software developed by RIKEN and Kobe University, and Project Chrono, an open-source vehicle motion analysis software. It can be applied to simulate the situation where vehicle motion and aerodynamic forces interact with each other. Moreover, the real driving environment where the wind fluctuations should be taken into consideration can also be conducted using the current framework. With this framework, we can assess the aerodynamic performance under the practical environment.

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Study on Foam Formation using Multi-phase-field Lattice Boltzmann Method with Adaptive Mesh Refinement

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Key Words: *Foam formation, Multi-phase-field, Lattice Boltzmann Method, Adaptive Mesh Refinement*

Foam formation is a common phenomenon that occurs daily, such as soap, beer, and sea foams. The phenomenon also occurs in various industries, such as textile, food, and oil recovery. Foam formation simulation is challenging because the liquid film separating gas bubbles is very thin compared to the bubble diameter, and the mechanisms to stabilize the foam formation are complicated. It is difficult to simulate the problem using conventional methods because of the finite resolution to resolve the thin film. As a result, bubble coalescence will occur when multiple interfaces are within a single computational cell, a phenomenon is known as numerical coalesce.

We simulate the foam formation using a multi-phase-field (MPF) lattice Boltzmann method (LBM) with adaptive mesh refinement (AMR). Using the MPF model, multiple bubble interfaces can be simulated within a single cell, preventing the numerical coalesce. The cumulant LBM is employed to simulate the hydrodynamics stably and efficiently using parallel computers. AMR is introduced to simulate the problem efficiently by concentrating the computational cells at the interface regions. The proposed method has been validated and used for large-scale simulation of foam formation with many bubbles. Several cases are simulated to gain insight into the behavior of the foam formation using various surface tension, bubble sizes, and viscosity. This study is expected to help understand the effect of foam formation on heat transfer in a medium in the future.

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Super-simulation of Coal Gasification Facility on Fugaku

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Key Words: *Coal Gasification, Combustion LES, Thermal Conduction and Cooling, Two-way Coupled Simulation, Supercomputer Fugaku*

In this research, we target one of innovative clean energy systems, i.e. carbon-free coal gasification plant. The coal gasification is one of the key technologies to drastically reduce CO_2 emission from coal fired power generation. Coal is crushed into fine particulate matter and then partially burned into gas in a high-pressure and elevated-temperature environment.

We perform a high-fidelity two-way coupled simulation of combustion turbulent flow and thermal conduction and cooling in a reactor vessel of a laboratory-scale coal gasification facility. We first explain our developed multiphysics and multiscale simulations on the Supercomputer Fugaku, which we call Super-simulation in short. Here a unique parallel coupler, REVOCAP_Coupler, is used to integrate highly parallelized independent solvers such as a FVM-based combustion LES flow solver, FFR-Comb, and a FEM-based thermal conduction and cooling solver, ADVENTURE_Thermal.

The simulation results are quantitatively compared with experimental results obtained from the laboratory-scale experimental facility. We succeeded in quantitatively reproducing the experimental phenomena in the facility with regard to temperature distribution as well as generated chemical components. The developed simulations will be powerful tools to improve the design and operation of actual coal gasification plants.

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Three-dimensional Flow Field Decomposition with Massively Parallel Distributed Learning on Fugaku

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Key Words: *Flow Field Decomposition, Machine Learning, Distributed Learning, Fugaku*

POD (Proper Orthogonal Decomposition) is the most typical method for decomposing the flow field into the modes [1]. However, since POD reduces the system's dimension by a linear function, it is known that sufficient reproduction accuracy cannot be obtained in a flow field in which advection is predominant, and non-linearity is prominent [2]. Therefore, Murata et al. used a convolutional neural network (CNN) to perform non-linear mode division for a two-dimensional flow field around a cylinder [3]. In this study, this network is expanded to three dimensions, and mode division is performed by large-scale distributed learning on Fugaku.

As a result, it was confirmed that if the time interval of the flow field snapshot data to be learned can be sufficiently small to resolve the oscillation with a short cycle, the reproduction accuracy of the detailed vortex structure of the flow field improves as the number of modes increases. In addition, it was confirmed that the computational performance in distributed learning on Fugaku scales well to about tens of thousands of nodes (million cores) by increasing the number of decomposing modes.

Based on the above results, by using the neural network used in this study, we demonstrate the possibility that the complex vortex structure and short cycle oscillation of a three-dimensional fluid can be reproduced with sufficient accuracy by adjusting the accuracy of the learning data and the number of modes. In the future, we would like to increase the scale of distributed learning further and aim to improve parallel computing performance to decompose with a sufficient number of modes required for the reproduction of the complex three-dimensional flow field.

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Tree Cutting Approach for Reducing Communication in Domain Partitioning of Tree-based Block-structured Adaptive Mesh Refinement

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Key Words: Adaptive Mesh Refinement (AMR), Static AMR, Lattice Boltzmann Method

We developed a block-structured static adaptive mesh refinement (AMR) CFD code for the aerodynamics simulation using the lattice Boltzmann method on GPU supercomputers. The data structure of AMR was based on the forest-of-octrees, and the domain partitioning algorithm was based on space-filling curves (SFCs) [1].

We evaluated the performance of the code and found that, in GPU computing, the SFC-based domain partitioning had a bottleneck on costly halo data communication. To reduce the halo data communication, we introduced the tree cutting approach (Fig. 1, Ref. [2]), which divided the global domains with a few octrees into small sub-domains with many octrees, leading to a hierarchical domain partitioning approach with the coarse structured block and the fine SFC partitioning in each block.

The tree cutting improved the locality of the sub-divided domain, and reduced both the amount of communication data and the number of connections of the halo communication. In the strong scaling test on the Tesla V100 GPU supercomputer, the tree cutting approach showed ×1.82 speedup at the performance of 2207 MLUPS (mega-lattice update per second) on 128 GPUs.

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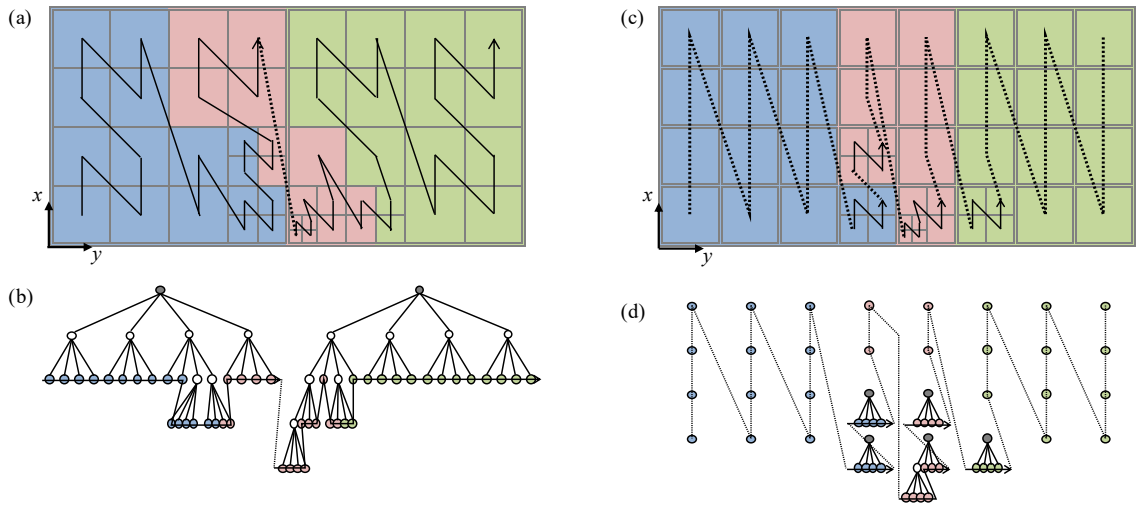

Fig 1: 2D example of domain partitioning in AMR. (a), (b) With conventional space-filling curve (SFC) approach. (c), (d) With tree cutting approach.

Voxel topology optimization of vehicle frame structure subject to multiple loading using building cube method framework

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Key Words: *Voxel topology optimization, High performance computing, Finite element method*

Topology optimization [1,2] is widely used in structural engineering design problems, including automobile frames. To obtain the conceptual structure of an automobile frame from a large area of metal blocks by topology optimization, we need a volume constraint of less than 1% and sufficient element resolution. The building-cube method (BCM[3]) with hierarchical Cartesian mesh has been developed for large-scale industrial simulations for fluid dynamics and also for fluid-structure interaction analysis[4].

Authors have developed a voxel topology optimization framework using finite element analysis under the BCM environment. Topology optimization of billions of elements intended for a vehicle frame subject to a single load case is performed using tens of thousands of processors, and its parallel performance is measured. In this paper, topology optimizations of automobile frame structure subject to multiple load cases are discussed. Torsional and bending load case is assumed to obtain a more robust and realistic design with various directional forces. The optimal shapes of a single load case and multiple load case are compared. Based on these results, we will discuss the characteristics of topology optimization itself that are necessary for the assembly-level manufacturing constraint function to be developed in the future.

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A performance portable implementation of high-order, entropy-stable spectral collocation schemes for compressible turbulent flow

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Key Words: high-order methods, high performance computing, fluids

High-fidelity simulations of compressible turbulent flows play a crucial role in the development of future technologies. Exascale computing will be a key component in enabling high-fidelity analysis and design but fundamental shifts in computing architectures have introduced challenges into how to best exploit modern hardware. High-order, matrix-free methods have the potential to dramatically improve the efficiency of these simulations by benefiting more from the high computational throughput on modern hardware compared to traditional second-order methods. Unfortunately, modern hardware is changing rapidly and refactoring a code to work efficiently on the latest hardware is becoming increasingly infeasible. In an effort to avoid architecture specific programming, software libraries such as Trilinos and programming models such as Kokkos are important to obtain performance portable implementations.

In this talk, we provide an overview of a performance portable implementation for high-order, entropy-stable spectral collocation schemes for tensor product elements through the use of Trilinos libraries and the Kokkos programming model. We introduce a preconditioned Jacobian-free Newton-Krylov method to drive unsteady simulations of turbulent compressible flow. We also provide a detailed performance analysis of the solver on various CPU and GPU architectures and compare our implementation with methods used for traditional finite volume schemes. We show that these high-order schemes perform better on modern hardware given a metric that includes both time-to-solution and error.

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Hyperdimensional, Adaptive Finite Elements Using Camellia and Intrepid2

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Key Words: High-order Finite Elements, Hyperdimensional Meshing, Adaptive Mesh Refinement, Plasma Physics, Vlasov Equation, Space-time Finite Elements

Camellia is a finite element library designed to facilitate rapid development of computationally efficient, hp-adaptive finite element solvers, starting with support for DPG. Intrepid2 is a package within Trilinos upon which Camellia depends for assembly. In Camellia, we have recently added support for meshes beyond 3D, with particular application to the Vlasov equation and space-time finite elements. Meanwhile, in Intrepid2 we have added data structures to support efficient storage of tensor-product data, and implementations of sum-factorized assembly built atop those structures. In this talk, we discuss these capabilities, as well as efforts to combat the curse of dimensionality, with some sample results from space-time Vlasov problems.

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On performance portability of physical problems using libCEED

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Key Words: Turbulent flows, CPU, GPU, High-order Finite/Spectral Elements, libCEED

Recent and emerging HPC systems change the balance of compute/memory/latency. This has fundamental consequences on choice of data structures and algorithms to accurately and efficiently solve physical problems. Although some existing software exploits structure in high order methods to achieve high performance on modern architectures, it usually comes with compromises such as special-purpose application, incidental complexity and debugging difficulties for users and developers, limited architectural targets, and complex packaging and distribution. libCEED is a new mathematical software library that offers flexible, performance-portable algebra for finite element operators and preconditioning. It offers a simple interface that readily handles real-world complexities such as implicit material models, stabilization/shock capturing techniques, and matrix-free multigrid without compromising performance on various computational device types. libCEED exploits structure in high-order finite/spectral elements in a lightweight package without environment assumptions. In this presentation, we investigate the effect of problem size, polynomial degree, parallelism, and physical complexity on the accuracy, cost, and execution time on CPU and GPU architectures for a variety experiments including compressible turbulent flows.

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A Comparison of Different Isogeometric Refinement Strategies for the Solution of 2D Hertzian Contact Problem

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Key Words: Hertzian contact, Isogeometric analysis, NURBS, Discretization, Refinement techniques

The finite element analysis (FEA) is considered one of the most popular numerical techniques used to get the solution of a Hertzian contact problem. However, one of its limitations is the utilization of approximate geometry, which causes geometric error in the analysis. This problem can be alleviated by the isogeometric analysis (IGA) technique [1]. This is because the technique uses spline technology to create geometric models. It also provides various refinement options, viz., order elevation, knot insertion, and a combination of the former two, i.e., $k-$refinement for geometric smoothness. The application of IGA to contact problems has gained popularity because of the deliverance of its accurate and robust predictions over FEA [2]. To the best of the authors' knowledge, a comparative assessment of refinement techniques in IGA is not available for the solution of contact problems and hence is the scope for present work. In this contribution, an investigation of several refinement techniques in IGA is presented for the solution of the 2D Hertzian contact problem. In combination with the Gauss-Point-to-Surface (GPTS) formulation, the penalty method is used to incorporate the contact constraints. It is validated that the order elevation and the knot insertion techniques in IGA imitate the $p-$ and $h-$refinement techniques in FEA, respectively. The accuracy of the results improves with the increase in the order of underlying basis functions or new knots in the knot vector, provided the geometry and parameterization are preserved. Further, the numerical results using knot insertion converge to the actual solution faster than the order elevation for each refinement step. The $k-$refinement technique, which utilizes an order elevation process followed by knot insertion, provides better results even with the coarse mesh resolution. The oscillations in the results using this technique reduce faster than the other two techniques. It is concluded that the order elevation and the knot insertion steps within the $k-$refinement technique can be incorporated in a controlled manner to optimize the computational cost and time.

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A Discrete Energy Consistent Approach for Implict Dynamic Contact with Displacement and Velocity Constraints

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Key Words: Implicit Dynamics, Contact, Stability

Standard time integration schemes such as Newmark's method are well known to have stability issues and chatter in the event of unilateral contact. This is due to inherent smoothness built into these time integration schemes and the lack of control of the energy due to the nonlinear nature of the impact. A large body of literature has been developed to treat these issues and a small survey of the different approaches will be presented. A number of approaches apply Lagrange multipliers and employ a velocity jump (e.g. [1, 2]) in the time integration scheme to handle impulse occuring at impact. Some employ incremental gap forms [3, 2] whilst others apply special techniques to enforce the explicit gap constraint at each time step [4, 5]. Some employ penalty constraints and balance energy at contact release [3]. Several incorporate special schemes to add algorithmic damping to mitigate high frequency noise [4]. This work combines different aspects from previous approaches, includes Lagrange multipliers and yields an algorithm that is provably B-stable in a discrete energy norm. Here, energy is dissipated at impact and the velocity is updated by applying a bilateral constraint to enforce persistency. This process is inherently dissipative but an additional force can be applied to recover the lost energy upon contact release if desired. In fact, the proposed conserving approach only requires two subsequent linear solves at the end of time step to recover lost energy as opposed to the nonlinear solve necessary in [2].

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A Reverse Constrained Preconditioner for the Lagrange Multipliers Method in Contact Mechanics

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Key Words: Contact mechanics, Lagrange multipliers, AMG

To accurately simulate the geomechanical response of a complex subsurface system, such as an aquifer or a hydrocarbon reservoir, it is critical to capture the behavior of faults and fractures. Several phenomena, such as micro-seismicity and fracture propagation, depend on the nature of these discontinuities. As a result, it is important to account for the complex behavior across these fractures explicitly. From a modeling viewpoint, it is necessary to simulate the influence of the fractures on the mechanical deformation. Dealing with frictional contact problems lies at the core of the challenge [1].

The frictional contact problem is one of the most challenging in the computational mechanics field, since it usually produces a stiff non-linear problem associated with a series of linear systems, that is hard to solve efficiently. We use Lagrange multipliers to enforce the constraint and we focus on two different discretization techniques, one of which is intrinsically stable, while the other requires a stabilization [2].

To solve the saddle-point Jacobian matrices arising from the linearization, we propose a constraint preconditioner where the primal Schur complement is obtained by eliminating the Lagrange multipliers unknowns. Suitable augmentation is presented for the intrinsically stable case. Finally, an optimal multigrid method [3] is applied to efficiently solve the Schur complement. We provide numerical evidences of the robustness and efficiency by solving large size problems from various applications.

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A Smooth Spline-based Contact Approach for Beams: Normal and Tangential Interactions

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Key Words: *Smooth Contact, Normal Interaction, Tangential Interaction*

A frequent strategy to model mechanical contact in a finite element context is to adopt the elements' geometry to formulate the contact interaction. This strategy, however, can lead to numerical difficulties due to ill-defined contact geometries such as sharp corners formed between straight finite elements. To avoid such issues, particularly in the context of beam-to-beam contact, this work proposes a spline-based C^1 continuous contact formulation, able to model beams with circular cross-section. The main advantage of this approach stems from a spline description which guarantees a smooth geometry of the whole structure. The proposed contact formulation starts from a classical finite element mesh that defines the spline control points and leads to a spline-based mesh that is employed to model the contact interaction. Moreover, a consistent strategy is developed to split the spline patches into specific elements, more suitable for the contact interactions. The normal gap definition is based on an approach, first presented in [1] and later expanded in [2] to a spline description. Once the contact scenario and the gap are defined, a nonlinear normal interaction law is introduced. A two-parameter general polynomial law is proposed for the nonlinear normal contact interaction with the objective of modeling a broad range of problems, including the linear penalty case. A normal damping (dissipative) contribution is also included. For the tangential interaction, a specific gap that is geometrically defined by the tangential projection of the relative displacement obtained from two consecutive contact configurations is adopted [3]. With the tangential gap established, a specific rheological model including two sliding devices is used [4] which includes an elastic and a dissipative contribution. Additionally, static and dynamic frictional interactions are considered in the rheological model. Several examples are solved that show the robustness and applicability of the proposed formulation.

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A Trust-region Method for solving finite deformation contact problems in Unfitted Finite Element Method

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Key Words: extended discretization methods, Lagrange mutliplier, multigrid method, contact problems

Unfitted methods simplify the cumbersome task of generating high-quality meshes that fits the computation domain explicitly. In the unfitted methods, structured background meshes are used and the underlying finite element spaces are modified to incorporate the geometrical details of the computational domain. In this work, we consider frictionless contact problems in the context of finite deformation and discretize this problem using an unfitted finite element method. We use the method of Lagrange multipliers to enforce the non-penetration contact condition, where the inf-sup stability of the discretization is ensured by employing the vital-vertex algorithm. Moreover, we also employ a variant of the ghost penalty term to control the gradients of the solution on the cut-elements.

Solving such contact problems in the finite-deformation framework requires minimization of nonlinear energy functional such that the non-penetration condition on the contact boundary is satisfied. Here, we propose to use the trust-region method to solve such a nonlinear constrained minimization problem. The proposed trust-region method provides convergence control and accommodates the constraints naturally in the algorithm. To solve the arising trust-region subproblems, we use a tailored generalized multigrid method that can tackle the linear inequality constraints and the point-wise constraints arising from the convergence control. We show the essential modifications for the smoother to handle the contact and the trust-region constraints, simultaneously. For the transfer operators, we use a so-called pseudo-L^2-projection which is designed specifically for the unfitted finite element framework. Lastly, the robustness and the efficiency of the proposed solution method will be demonstrated and a comparison with the other methods will be made.

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An implicit beam to shell contact algorithm using corotational beam elements and rotation-free shell formulation for vascular biomechanics

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Key Words: *Contact, Corotational Beam, Rotation-Free Shell, Cardiovascular*

The mechanics of beam-to-surface contact has important applications in cardiovascular minimally invasive surgery (carotid and intracranial stents, catheters, guide-wires and coils, stent-retrievers for acute stroke treatment, venous filters and other devices to treat venous thrombosis). Surgical planning is still sub-optimal at the patient-specific level and there is a pressing need to provide surgeons with in-silico patient-specific models capable of capturing the complex mechanics of the contact between the device and the vessel. On top of this, the stringent clinical time frame calls for efficient algorithms, able to provide accurate simulations in a short time.

This article builds upon our previous work in rotation-free shell elements [1] and beam to surface contact using corotational beams [2]. The formulation presented in [1] exploits the fact that the thickness to radius ratio of vascular vessels is relatively small and therefore, they can be accurately modelled using shell elements. The rotation-free shell element calculates both the membrane and bending behavior via displacement degrees of freedom for a triangular element, resulting in an efficient formulation to model complex patient-specific geometries while incorporating biologically relevant 3D hyperelastic constitutive models. In [2], the authors presented an efficient beam to rigid surface contact formulation using corotational beam elements. Such elements allow to decompose the deformation into rigid body rotations and small local deformations, which results into an efficient formulation as compared to Total Lagrangian beam models.

This work presents a fully implicit algorithm that couples the contact between the corotational beam element and the rotation-free shell formulation. The new contributions are fully linearized to update the tangent operator and the system is integrated in time via the HHT-α method. The algorithm is implemented using Julia within an on-going open-source development. Overall, a consistent implicit contact dynamics formulation is obtained. Several examples are provided to illustrate the accuracy and robustness of the proposed algorithm.

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An interface-enriched generalized finite element formulation for locking-free coupling of non-conforming discretizations and contact

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Key Words: Enriched FEM, IGFEM, non-conforming meshes, contact, Lagrange multipliers, multiple-point constraints

We propose an enriched finite element formulation to address the computational modeling of contact problems and the coupling of non-conforming discretizations in the small deformation setting. The displacement field is augmented by enriched terms that are associated with generalized degrees of freedom collocated along non-conforming interfaces or contact surfaces. The methodology follows from our previous work on the Interface-enriched Generalized Finite Element Method [1, 2]. The enrichment strategy effectively produces an enriched node-to-node discretization that can be used with any constraint enforcement criterion; this is demonstrated with both multiple-point constraints and Lagrange multipliers, the latter in a generalized Newton implementation where both primal and Lagrange multiplier fields are updated simultaneously. The *node-to-node enrichment* ensures continuity of the displacement field—without locking—in mesh coupling problems, and to transfer fairly accurate tractions at contact interfaces—without the need for contact stabilization—is demonstrated by means of several examples. In addition, we show that the formulation is stable with respect to the condition number of the stiffness matrix by using a simple Jacobi-like diagonal preconditioner.

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Consequences of third-body thickness on first-bodies

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Key Words: *third-body, fretting, friction, flow regime, contact*

Fretting is a tribological phenomenon generated by two parts in contact, called first-bodies, undergoing a relative movement of small amplitude. In some dry contacts, as in the case of fretting, the relative motion between the two first-bodies generates third-body particles. This third body plays several roles in the life of the contact and notably participates in transmitting loads and accommodating velocities [1]. The understanding of the influence of the third body flow is a prerequisite to the writing of wear models taking into account the entire tribological triplet, constituted of the two first-bodies, the third body, and the loading system.

The MELODY software, developed at LaMCoS [2], allows modeling the third body (Figure 1). Between two bodies, one rigid and the other deformable, a collection of deformable grains is generated, then subjected to normal pressure and shear. Numerical results show that the third body can present several aspects and flow according to several regimes (plastic, granular, agglomerated, etc.) depending on the values assigned to two parameters: stiffness and cohesion between particles. These different flow regimes greatly influence the stresses undergone by the first bodies and therefore their wear. During the lifetime of the contact, the thickness of the third body can vary greatly. We thus ran a campaign of numerical simulations in order to analyze the influence of the third-body thickness on the stresses undergone by the first bodies, and on their variations in time and space.

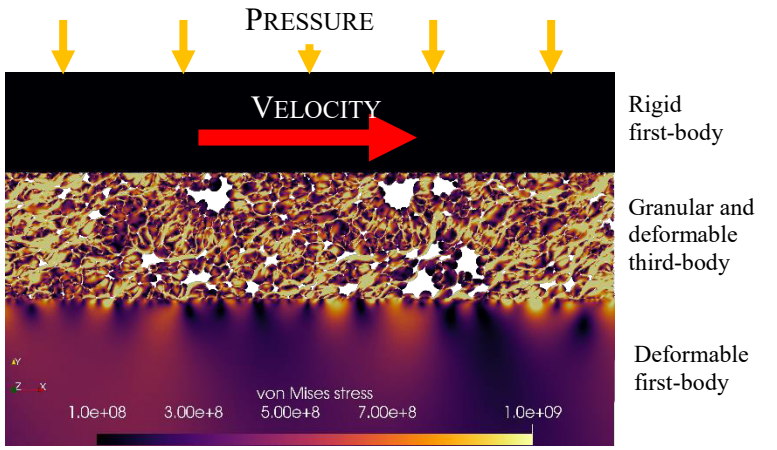

Figure 1 : Simulation with 700 deformable particles submitted to compression and shear. The lower body is deformable. The color indicates the constraints of von Mises.

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Consistent Coupling of 1D Cosserat Beams and 3D Solid Bodies: From Embedded Fibers Towards Contact

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Key Words: *Nonlinear Beam Theory, Contact Mechanics, Mixed-Dimensional Coupling*

In this contribution, we first present a consistent coupling method for fully embedding arbitrary curved one-dimensional (1D) Cosserat continua (i.e., beams) into three-dimensional (3D) solid volumes, as e.g., in fiber-reinforced materials [1]. The beams are explicitly modeled with 1D geometrically exact beam finite elements, while the surrounding solid volume is modeled with 3D continuum (solid) elements. The translational and rotational degrees of freedom of the beams are coupled to the solid, thus requiring a suitable definition of a representative rotation tensor field within the solid domain [2]. An objective, i.e., frame invariant, embedded mortar-type approach is presented to enforce the kinematic coupling constraints between the beam and solid elements on inevitably non-matching and mixed-dimensional meshes. We demonstrate optimal rates of spatial convergence and showcase the capabilities of the proposed method for various applications.

As a second step towards increasingly complex beam-to-solid interaction scenarios, the mortar-type coupling approach is extended to the 1D-2D case, i.e., the attachment of beams onto solid surfaces, well-known from biomedical devices such as endovascular stent grafts. Additional challenges arise due to the natural existence of a discrete field of surface normal vectors, which must be properly dealt with when formulating the coupling constraints to avoid unphysical internal stresses and to guarantee exact conservation of both linear and angular momentum.

Finally, our recent research efforts regarding the most general beam-to-solid interaction scenario of unilateral contact are highlighted. While beam-to-solid volume coupling and beam-to-solid surface coupling could rely exclusively on a consistent formulation in the undeformed reference configuration, we must now carefully consider finite deformations and relative motions including finite sliding of beams across solid surfaces. Consistent linearization and its crucial importance for nonlinear solver robustness within implicit dynamics as well as the use of various state-of-the-art discretization techniques for the solid bodies, e.g., NURBS-based isogeometric analysis [3], will be illustrated along with challenging applications from engineering practice.

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Dynamic load balancing for contact mechanics at large scale

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Key Words: Contact Mechanics, Mortar Methods, High Performance Computing, Domain Decomposition, Finite Elements

Computational contact mechanics provide insight into various physical phenomena, e.g. frictionless contact, frictional sliding, or wear problems just to name a few. Although mortar methods [1] are widely considered the favorite approach due to their variational consistency, high accuracy and outstanding robustness, the accurate evaluation of mortar terms and their linearizations comes at a high computational effort and cost. While we have already proposed scalable iterative solvers for contact problems [2], the cost for evaluating the mortar terms might become dominant or even prohibitive at large scale. While the parallelization of the finite element evaluation is well established to speed-up simulations, the evaluation of mortar terms requires special care in a parallel computing environment.

In this presentation, we study the impact of the curse of dimensionality onto the overlapping domain decompositions of the volume and interface discretizations and its effect on parallel scalability and the overall time to solution. As a remedy, we then develop load balancing schemes for static and dynamic contact problems to optimally distribute computational work to all available hardware resources of parallel computing clusters [3]. Furthermore, we outline a geometrically motivated ghosting strategy based on cartesian bins to reduce the storage and parallel communication of the master side of the contact interface. We demonstrate weak and strong scalability of the proposed algorithms in the context of three-dimensional static and dynamic contact problems and discuss load balancing and ghosting strategies for various practical scenarios.

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Effect of particles on contact model under three-body contact conditions

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Key Words: *Wear particle, Contact mode, Friction, Interface*

Methodology:
This paper studies the effect of the diameter and the number of the wear particle on the contact mode and friction coefficient at the contact interface under 3-body contact conditions. When the particle and two surfaces are in contact under the 3-body contact conditions, the friction coefficient (μ_s) is the sum of surface-to-surface friction (μ_{ss}) and surface-to-particle friction (μ_{sa}) of solid contact, which can be calculated from three-body friction model [1]. The main cause of wear on the contact surface is the solid friction, so the contact behavior at the interfaces can be obtained from the changes in the surface contact area (A_{ss}) and particle contact area (A_{sa}) [2]. The results of an extensive set of simulations are then used to obtain the curve-fit expressions for the film thickness [3,4].

Results:
The results show that the friction coefficient increases with increasing particle diameter (x_a) and the number of particles per unit area (η_a), and decreases with increasing speed parameter (U). When the wear debris is too large or its concentration is too high, the contact model of the interface is easily transferred into the 3-body S-P contact model, which can produce an excessive friction coefficient. Controlling the size and concentration of wear debris can effectively increase the lifetime of components.

Conclusions:
This paper estimates the tribological performances of interface contacts using a 3-body contact model. The effects of size and concentration of particles on the contact model are analyzed. The proposed 3-body model is validated by comparing to the results obtained from the other existing model. This work is helpful to understand the contact mechanism transitions, the wear process during running-in in mechanical components, as well as the mixed lubrication mechanisms.

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First-order Primal-dual Algorithm for Quasi-static Unilateral Contact Problem with Coulomb Friction

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Key Words: Coulomb Friction, Complementarity Problem, First-order Method, Second-order Cone

Recently, accelerated first-order methods have received significant attention for solving large-scale optimization problems in data science. First-order methods do not use the second derivatives of the functions in an optimization problem, and their computational cost per iteration is cheap. By incorporating an acceleration scheme, the number of iterations required by a first-order method can be reduced considerably [4]. Such an accelerated first-order method may possibly be efficient also for diverse problems in computational mechanics. For instance, it was demonstrated through the numerical experiments that an accelerated proximal gradient method developed for elastoplastic incremental problems outperforms a conventional second-order optimization method [5]. The author proposed an accelerated Uzawa method for frictionless contact problems [3].

This paper presents an accelerated first-order method for quasi-static problems with the unilateral contact and the Coulomb friction. The method is designed based on a primal-dual algorithm [1]. Major computational efforts for each iteration is solution of a system of linear equations and projections of variables onto the friction cones. We use a preconditioned conjugate gradient method for the former. The latter can be highly parallelized. It is shown in the numerical experiments that the proposed method outperforms a regularized and smoothed Newton method for second-order cone complementarity problems [2].

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New fast numerical technique for the resolution of the quarter space contact problem

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Key Words: Quarter Space, Edge, Semi-Analytical Method, SAM, Contact Mechanics

The elastic quarter space problem is commonly encountered in practical mechanical systems such as the contact of rail wheels, cam followers, gears and roller bearings. In these mechanisms the contact limit is so close to the free edge that the edge effects cannot be neglected or ignored. Another situation where edge effects modify the materials response is in the nanoindentation or indentation test (where the mechanical properties of the samples are sought up to the ends of the free edges). For these different contact cases, the Hertz assumptions are no longer valid, so a quarter space model enables to better translate the physical reality. The quarter space problem was first investigated by Shepherd [1]. This problem is very difficult and complex to solve analytically, several techniques have been developed by researchers. Among them Hetenyi [2] ingeniously proposed a technique of overlapping half space, which allowed to obtain an approximate numerical solution with an acceptable precision. Inspired by the Hetenyi's technique Guilbault [3] has proposed a new method of resolution. This paper presents a new quick and convenient method for solving the finite space problem based on the Guibault's method. Its validation was carried out by comparison with the finite element method and the literature.

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On the Application of Acceleration Techniques to a Partitioned Solution Approach to Thermomechanical Contact

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Key Words: *Thermomechanical Contact, Mortar Method, Acceleration Techniques, Partitioned Solution*

Thermomechanical coupling is of the most relevant multi-physics problems from the perspective of mechanical engineering. When contact is involved, the coupling emerges from the heat transfer across the contact zone and the dissipation of the frictional work into heat. As a result, the temperature evolution can trigger harmful changes in the material and interface properties, for instance, softening of the surrounding material and variations of the coefficient of friction. The wide range of applications that call for predictions on thermomechanical contact problems has fostered several investigations in the topic over the last decades. Solution approaches to this class of problems can be divided into monolithic and partitioned solutions. Monolithic schemes have superior stability and robustness, at the cost of higher complexity in the construction and solution of the system of equations [1]. On the other hand, (strongly) partitioned solution schemes provide significant simplifications of the implementation and may take advantage of several numerical techniques already developed for mechanical and thermal problems. However, this approach may lack convergence properties, namely concerning the iteration between fields [2]. This pitfall of partitioned solution strategies has motivated the development of acceleration techniques for coupled problems, typically studied in the absence of contact interaction [3].

Leveraging the significant body of literature on these techniques, we aim to accelerate the partitioned solution of thermomechanical contact problems. The state-of-the-art literature identified relevant convergence acceleration techniques based on the ease of implementation in partitioned solution schemes and numerical performance. These strategies are implemented in the in-house partitioned nonlinear finite element solver, equipped with a mortar-based discretisation of contact. The computational efficiency of each candidate is benchmarked using numerical examples with varying degrees of thermomechanical coupling at the contact interface. The present work enables the identification of advantageous alternative solution procedures for coupled contact interaction, that recover the solution of the monolithic approach, retain the simplicity of the partitioned schemes and exhibit competitive computational cost.

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Plastic zone analysis of nanoindentation for unique constitutive properties of elastoplastic materials

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Key Words: *Nanoindentation; Plastic Zone; Dimensionless Analysis.*

Nanoindentation has been used to evaluate the mechanical properties of the bulk, coating, or film materials at micro- and nano-scales as an advanced mechanical testing technique. Accurate and continuous measurements of the applied load on the indenter can be achieved at micro-Newton accuracy as a function of the indentation depth at the nanometer level. The major advantage of the depth-sensing indentation technique is the lack of requirements for the size and geometry of the material samples. Indentation experiments have been performed to evaluate mechanical properties and residual stresses of various types of materials. The nanoindentation responses from different types of indenters are closely associated with the elastoplastic stress–strain responses of isotropic materials.

It is challenging to describe the evolution of the plastic zone underneath the indenter during nanoindentation, and it is recently known to be crucial to establish a constitutive model that features the plastic properties of the substrate materials based on their indentation responses. Using molecular dynamics and axisymmetric finite element (FE) simulations in this study, we show that the plastic zone shape in the elastoplastic materials under a three-sided pyramide-shaped Berkovich indenter is hemispherical in a broad range of length scales. Dimensional analysis is performed to derive dimensionless functions regarding the radius of the hemispherical plastic zone, considering the critical factors of the load–penetration depth (P–h) curve. By focusing on the loading and the complete unloading stages after completing extensive FE simulations, polynomial functions are proposed by associating the instantaneous and residual plastic zone radii with constitutive parameters, such as Young's modulus, the hardening exponent, and the ratio of the representative stress and the reduced modulus.

As the main objective of this work, we discussed the use of the proposed dimensionless functions to obtain the unique constitutive properties of materials, especially the plastic parameters. We used three reverse algorithms to demonstrate that three elastoplastic materials with similar P–h curves could have significantly different plastic properties. The predicted P–h curves and stress–strain relationships indicated that slight differences in the P–h curves led to significant differences in the stress–strain relationships for all three reverse algorithms. The plastic zone radius represents a crucial parameter in the reverse analysis for predicting the unique plastic parameters of materials. Thus, the proposed dimensionless function of the residual plastic zone radius is essential to obtaining the relation between the evolution of the plastic zone radius and the unique plastic parameters of materials.

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The eXtreme Mesh deformation approach (X-MESH) for sharp contact fronts modeling

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Key Words: X-MESH, contact mechanics, variational inequality, membrane, sharp interface

Contact problems are governed by inequality constraints, which have been at the core of many research during the past decades [1, 2]. Most of these methods are quite efficient in modeling the inside of the contact zone, however only a few of them are able to sharply model the contact front (contact zone boundary). Yet, a sharp representation of the contact front is necessary to get optimal convergence rate, as it was shown by [3] for instance.

In this work, an efficient way to model sharp contact front is proposed, based on the X-MESH approach which was originally introduced in [4] to model phase-change fronts. The key idea is to move the nodes of a finite element mesh to have a time continuous, sharp representation of the contact front. These nodes movements allow to model topological change of the contact front, including coalescence and splitting, without remeshing or changing the mesh topology. Some finite elements may eventually reach zero measure, but we show in this work that this can be properly tackled.

The method could be applied to any contact problems, but we chose to illustrate its capabilities on several 1D and 2D quasi-static membrane problems in small perturbation. In particular we show that the X-MESH method allows to recover optimal mesh convergence rates, and how it allows to model complex topological changes of the contact zone.

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Added-mass of a finite length flexible cylinder in a narrow coaxial cylindrical duct

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Key Words: Vibration modes; Fluid-Structure Interaction; Added-mass; Coaxial cylinders, Narrow annulus

This work deals with the fluid-structure interaction problem of two coaxial cylinders separed by a thin fluid layer. The inner cylinder is flexible and is imposed a displacement corresponding to the vibration mode of an Euler-Bernoulli beam. Assuming a narrow duct as in [1], we carry out a new theoretical approach to obtain an analytical expression of the fluid added-mass matrix. This new formulation applies to finite size cylinders and encompass all classical types of boundary conditions. We show that the coefficients of the matrix depend on the aspect ratio of the flexible cylinder, the confinement of the duct and the characteristics of the imposed vibration mode.

To assess the validity of the theoretical predicitons, we perform numerical simulations with the open-source code TrioCFD [2]. In this code, the fluid-structure interaction problem involving moving boundaries is solved using an Arbitrary Lagrange-Eulerian technique. We show that the theoretical predictions are successfully corroborated by the numerical simulations, for all types of classical boundary conditions, for different confinements, and for different aspect ratios of the vibrating cylinder.

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Simplex Space-Time Finite Elements for Fluid-Structure Interaction

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Key Words: Simplex Space-Time Finite Elements, Fluid-Structure Interaction

In engineering, phenomena of fluid-structure interaction play an important role. A prominent example is aeroelasticity, where, e.g., the behaviour of elastic airplane wings has to be included in the design process in order to maximize the aerodynamic performance. But not only in aerospace engineering, also in other engineering areas one can find further examples: the blood flow through flexible arteries in bio-engineering, the deformation of wind turbine blades in energy engineering, the flexible hulls of ships exposed to wind and water in naval engineering, or the movement of flexible piston rings in automotive engineering.

In the presented work, the coupled problem is solved by time-continuous stabilized space-time finite element methods. Building on previous studies on time-dependent flow problems [1], the time-continuous simplex finite elements (C-SST) are applied on the fluid side, using an unstructured triangulation of the space-time domain. Following a boundary-conforming approach, the deformation of the coupling interface is treated via a pseudo-elastic approach [2]. On the solid side, we focus on simplified models, i.e., rigid-body or beam models, solved in the manner of time-continuous prismatic space-time finite elements (C-PST), where the spatial discretization is extruded in time, leading to a structured discretization in time. The overall solver is presented along with numerical results to underline its potential.

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Simulation of Interacting Deformable Particles at Low Reynolds Numbers Using Isogeometric Divergence-Conforming Immersed Boundary Method

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Key Words: FSI, Isogeometric Analysis, Immersed Boundary Method, Microswimmers

According to Purcell's scallop theorem, microswimmers need to break the time-reversal symmetry to achieve net body motion in a Newtonian fluid at low Reynolds numbers. For biological microswimmers, this is typically achieved through changes in their body shape, using flagella locomotion or, more commonly, combining both [1]. For artificial microswimmers made of interacting individual particles, the time-reversal symmetry is broken through cycles of non-reciprocal variations of the relative distances between particles. Numerical simulations of this type of microswimmers are carried out in very recent works with simplistic models, assuming far-field flow interaction between particles and representing the fluid through the Oseen's tensor [2]. In this work, we solve the fluid-structure interaction (FSI) problem with the Isogeometric Divergence-Conforming Immersed Boundary Method (IDCIBM) [3], where we include the Navier-Stokes equations for the description of the fluid motion and the constitutive equations of a Neo-Hookean material for the solid phase. The interactions between particles are controlled from the software package ESPResSo [4], taking advantage of its wide variety of already implemented short and long-range interacting forces. In the IDCIBM the Eulerian velocity-pressure pair is discretized using divergence-conforming B-splines, which leads to inf-sup stable, H1-conforming, and pointwise divergence-free Eulerian solutions. This numerical approach allows us to simulate microswimmers made of interacting deformable particles with no restriction on the separation distance. Furthermore, the methodology includes deformable particles, which is one more step to more realistic simulations.

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Tuft flow visualization and measurement

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Key Words: *Fluid-structure interaction, Tuft Visualization, Inverse problems*

A tuft is a strip of yarn or string attached to an aircraft wing or a car surface. Tuft flow visualization is a broadly used technique for capturing the flow pattern around an object and studying the dynamics of a fluid system [1]. This study aims to recover the velocity magnitude and direction of fluid flow from the deformation of a tuft. The deformation of the tuft depends on the geometry, material properties, and applied forces. Applied forces are related to the velocity of the fluid. An ABS (acrylonitrile butadiene styrene) strip was used as a tuft, and its deformation was measured. The experiment was conducted in an open water flume, and the deformation was measured by comparing images. The experiment was also simulated using a two-way coupled fluid-structure interaction model [2]. The tuft was modeled as a nonlinear shell (large deformation). The computational model was validated, and a series of experiments were developed to correlate the fluid velocity and the tuft deformation. Furthermore, the validated simulation was used to analyze a series of conditions varying by tuft geometry and fluid velocity. These results were used to create a regression model that determines velocity based on deformation. Preliminary results show that the velocity of a fluid flow increases nonlinearly as the deformation of the ABS tuft increases. It can also be observed that the regression model has a range of accuracy, and outside this range, the results are not reliable. On the other hand, using a variety of geometries and materials simultaneously increases the model's validity range.
Measuring the velocity of a fluid based on deformation enables measurements to be taken more efficiently in a variety of conditions. For example, in remote areas of the world where the equipment to measure wind speed is not available, or in the case of plumbing where measuring the velocity in pipes requires invasive equipment.

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Water Wave Interaction with a π-shape Floating Breakwater by Scaled Boundary FEM

Abstract

The principal aim of the current study is to examine a Scaled Boundary Finite Element Method (SBFEM)-based model to analyze the interaction problem between the water waves and moored floating breakwaters with sharp edges. Regarding the increasing employ of rectangular cross-section floating breakwaters with vertical side plates to their down-wave and up-wave sides (π-shaped floating breakwaters), they are used as a practical basis to examine how the model works. By comparing the present solutions to those from existing literature, without changing the mesh density compared to previous simulations used in simple configurations, the accuracy and generality of the present model in the complex configurations are evaluated. It is demonstrated that as the proposed model is a semi-analytical method, unlike conventional numerical methods, there is no need to refine the mesh around sharp corners, which can considerably save the computational time, effort, and cost in large solution domains.

Keywords: Scaled Boundary Finite Element Method (SBFEM), Floating Breakwaters, Wave Interaction, Water Wave Radiation, Water Wave Diffraction

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A Residual based a Posteriori Error Estimators for Algebraic Flux Correction Scheme

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Key Words: A posteriori estimator, Steady-state convection-diffusion equations, Algebraic flux correction (AFC) schemes, SUPG finite element method, Energy norm

Non-linear discretizations are necessary for convection-diffusion-reaction equations for obtaining accurate solutions that satisfy the discrete maximum principle (DMP). Algebraic stabilizations, also known as Algebraic Flux Correction (AFC) schemes, belong to the very few finite element discretizations that satisfy this property. Results regarding the convergence of the scheme [1] and efficient solution of the nonlinear system of equations [2] have been obtained recently..

The talk is devoted to the proposal of a new residual based a posteriori error estimator for AFC schemes. We derive a global upper bound in the energy norm of the system which is independent of the choice of the limiter in the AFC scheme. We also derive a global upper bound by combining the estimators from [3] and the AFC schemes. Numerical simulations in 2d are presented which support the analytical findings.

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A Volumetric Extrapolation Method for Weak Imposition of Interface Conditions on Level Sets

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Key Words: Unfitted FEM, Level Sets, Approximate Delta Functions, Shifted Boundary Method

We introduce a new way to implement Dirichlet, Neumann, or flux boundary conditions on level sets of approximate distance functions. The proposed approach can be interpreted as a diffuse interface version of the shifted boundary method (SBM) for continuous finite element discretizations of conservation laws on unfitted meshes [2, 3]. We impose the interface conditions weakly by substituting them into surface integrals, which we approximate by volume integrals (as in continuum surface force (CSF) implementations of surface tension in finite element level set methods for incompressible two-phase flows [1]). The calculation of volumetric interfacial terms requires (i) construction of an approximate delta function [5] and (ii) extrapolation of the immersed boundary data into quadrature points. We accomplish these tasks using a level set function, which is given analytically or evolved using the algorithm proposed in [4]. A globally defined averaged gradient of this approximate distance function is used to find the nearest point on the implicitly defined interface. The normal and tangential derivatives of the numerical solution at that point are calculated using the interface conditions and interpolated values. As in classical SBM approaches, extrapolation back to the quadrature points is performed using Taylor expansions. Numerical results are presented for a suite of new 2D test problems with fixed and moving interfaces.

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Elasto-Plastic Shock Dynamics using Implicit Shock Fitting with Space-Time Finite-Element Formulation

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Key Words: *High-order Finite Element Method, Space-Time, Discontinuous Galerkin, Shock Dynamics, Solid Mechanics, Implicit Methods, Unconstrained Minimization, Regularization*

Accurate and robust high-order discontinuous finite element formulations and numerical implementations for flows with discontinuities is a long-standing challenge, which so far has not been resolved satisfactorily. All known methods use shock-capturing, and require introduction of numerical diffusion to regularize the solution in the vicinity of discontinuities, typically in the form of ad-hoc filtering algorithms, non-linear limiters, hyper-/entropy-viscosity, flux-corrected procedures, etc. Recently, a new approach has been developed in [1], named the "*Moving Discontinuous Galerkin with Interface Condition Enforcement*" (MDG-ICE). MDG-ICE is designed to avoid using numerical dissipation, by incorporating the mesh motion into the global non-linear implicit iterative procedure. The method is capable of implicitly resolving wave patterns, detecting solution and derivative discontinuities and "fitting" the mesh to align with such solution features. This enables construction of a truly high-order discontinuous finite-element framework.

In this work, we focus on an extension of the MDG-ICE method to represent shocked solid dynamics. The response of solids is represented with an appropriate closure equation for the Cauchy stress tensor in a hypoelastic formalism. This work considers the Jaumann corotational stress rate [2]. The main challenges are the derivation of jump conditions for non-conservative deviatoric stress equations and how to properly incorporate plasticity effects. We show that our MDG-ICE discretization of this solid dynamics model is capable of delivering exceptionally accurate solutions. A set of 1D-in-space (2D space-time) test problems [2,3] featuring the interaction of solid rods (fliers) with elasto-plastic shock responses are demonstrated, as well as an initial demonstration of 2D-in-space (3D space-time) Taylor anvil impact.

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Exact Representation of Curved Material Interfaces in High-Order Lagrangian Hydrodynamics

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Key Words: Shock hydrodynamics, Shifted boundary method, Multi-material, Lagrangian/Eulerian/ALE, interfaces

We present a new algorithm for high-order numerical simulations of multi-material Lagrangian hydrodynamics. The discretization is based on the finite element method by [Dobrev et al, SISC, 2012], which is combined with the idea of the shifted interface approach, originally proposed in [Scovazzi et al., Int J Numer Methods Eng., 2019]. The proposed interface representation provides three major properties. First, the material interface is represented as a sharp jump, i.e., there is no artificial material mixing in the interface region. Second, the curved interface is obtained without any computations in cut elements or similar geometry-based calculations. This allows to maintain the computational efficiency and generality of the finite element discretization. Third, the method can achieve high-order convergence when the flow around the interface is smooth.

The shifted interface approach falls into the category of immersed/embedded finite element methods. Integrals over the material interface are approximated by integrals over surrogate mesh faces. These face integrals take into account the distance between the positions of the interface and the face. This distance is represented as a global high-order finite element function whose zero level set represents the material interface. The distance function is advected with the material velocity, resulting in representation of curved interfaces inside curved mesh elements. In the limit of fitted interfaces, the additional integrals disappear. We will present initial results on standard 2D and 3D benchmarks, obtained by our extension of the Laghos shock hydrodynamics mini-application.

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Invariant-Domain Preserving Approximations for the Euler Equations with Tabulated Equation of State

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Key Words: Compressible Euler equations, tabulated equation of state, maximum wave speed, Riemann problem, Invariant-domain preserving approximation, composite waves

This work is concerned with the approximation of the compressible Euler equations supplemented with an equation of state that is either tabulated or is given by an expression that is so involved that solving elementary Riemann problems is hopeless. A robust first-order approximation technique that guarantees that the density and the internal energy are positive is proposed. A key ingredient of the method is a local approximation of the equation of state using a covolume ansatz from which upper bounds on the maximum wave speed are derived for every elementary Riemann problem. This work is documented in [1].

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3D coupled FSI analysis for passive morphing adaptivity in Wells turbine

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Key Words: Multi-Scale Problems, Multiphysics Problems, Fluid Structure Interaction, Turbomachinery, Wells Turbine, Wave Energy

A 3D Fluid Structure Interaction (FSI) unsteady simulation is performed using Finite Elements Method and a strongly coupled approach with an in-house built software on a flexible Wells turbine blade.
Flexible blades could represent a practical and promising technological solution to enhance the performance of Wells turbines, by passively adapting the shape of the blade profile to the alternating direction of the air flow in a Wells turbine for an Oscillating Water Column plant. Additionally, the adoption of flexible blades in air turbines could lower the cost of the manufacturing process by selecting low-cost materials, and consequently reduce the cost per kilowatt of the device.
The main objective of the paper is to propose a design of a Wells turbine with flexible blades, inspired by boat sails, by observing and exploiting the passive morphing behaviour of thin structures in immersed high Reynolds flows. To achieve that, we perform a 3D FSI simulation of a Wells turbine with flexible blades.
A secondary claim of the work is to evaluate the dynamic response of the structure, as well as the eventual occurrence of unexpected aeroelastic effects due to the positive feedback between the fluid and the structure. The analysis can provide useful insights both about the feasibility of the proposed design and about the performances of the proposed flexible blades with respect to the classical technology.
The simulations are carried out using the Residual Based Variational MultiScale (RBVMS) method to solve the Navier-Stokes equations, the Total Lagrangian formulation (TL) for the structural non-linear elastic problem, and the Solid Extension Mesh Moving Technique (SEMMT) to move the mesh and avoid a continuous remeshing of the computational domain.

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A (Weighted) Shifted Boundary Method for Moving Boundary Problems

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Key Words: Shifted Boundary Method, Embedded finite elements, unfitted finite elements, immersogeometric finite elements

The Shifted Boundary Method (SBM) belongs to the class of unfitted (or immersed, or embedded) finite element methods and was recently introduced for the Poisson, linear advection/diffusion, Stokes, Navier-Stokes equations, and many additional problems [**?**, **?**]. By reformulating the original boundary value problem over a surrogate (approximate) computational domain, the SBM avoids integration over cut cells and the associated problematic issues regarding numerical stability and matrix conditioning. Accuracy is maintained by modifying the original boundary conditions using Taylor expansions. Hence the name of the method, that *shifts* the *location* and *values* of the boundary conditions. When considering the application of the SBM to incompressible flows with moving boundaries or free surfaces, spurious pressure oscillations in time may result from a discrete change of the total volume of active fluid over a time step. To avoid this issue, a weighted SBM is proposed, in which the variational form of the equations is weighted by the elemental volume fraction of active fluid [**?**]. The proposed weighted SBM (or W-SBM) induces small mass (i.e., volume) conservation errors, which converge quadratically in the case of piecewise-linear finite element interpolations, as the grid is refined. We present an extensive set of two- and three-dimensional tests to demonstrate the robustness and accuracy of the method.

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A Hyperelastic Extended Kirchhoff–Love Shell Model with Out-of-Plane Normal Stress

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Key Words: Kirchhoff–Love shell model, Hyperelastic material, Out-of-plane normal stress, Out-of-plane deformation mapping, Neo-Hookean material model, Fung's material model

A shell formulation based on the Kirchhoff–Love shell theory and isogeometric discretization was introduced in [1]. It has the advantage of not requiring rotational degrees of freedom. Extension to general hyperelastic material can be found in [2, 3]. We are introducing a hyperelastic extended Kirchhoff–Love shell model with out-of-plane normal stress. We present the derivation of the model, with focus on the mechanics of the out-of-plane deformation. To determine the out-of-plane stress, we solve the linear-momentum-balance equation in the out-of-plane direction. Accounting for the out-of-plane normal stress distribution in the out-of-plane direction affects the accuracy in calculating the deformed-configuration out-of-plane position, and consequently the nonlinear response of the material. The improvement is beyond what was achieved with the new model's precursor [3] by accounting for the out-of-plane deformation mapping. By accounting for the out-of-plane normal stress, the traction acting on the shell can be specified on the upper and lower surfaces separately. With that, the new model is free from the "mid-surface" location in terms of specifying the traction. We also present derivations related to the variation of the kinetic energy and the form of specifying the traction and moment acting on the upper and lower surfaces and along the edges. We present test computations for plate bending, plate saddle deformation, and pressurized cylindrical and spherical shells.

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A Unified Framework of Navier-Stokes Cahn-Hilliard Models with Non-Matching Densities

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Key Words: Navier-Stokes Cahn-Hilliard equations, mixture theory, thermodynamic consistency

Over the last decades, many diffuse-interface Navier-Stokes Cahn-Hilliard (NSCH) models with non-matching densities have been proposed, see e.g. [1, 3, 4]. Even though these models claim to describe the same physical phenomena, they are distinct from one another. The aim of this talk [2] is to present a unified framework of NSCH models that brings all of these models together. The core principles of the framework are the following:

1. there is only one system of balance laws based on continuum mixture theory that describes the physical model.
2. there is only one natural energy-dissipation law that leads to quasi-incompressible NSCH models.
3. variations between the models only appear in the constitutive choices.

We additionally aim to indicate and rectify inconsistencies of existing volume-averaged velocity based models with respect to mixture theory. Furthermore, we identify the mobility to be of degenerate type and show that a non-degenerate mobility leads to an incompatibility in the limit of the single-fluid regime.

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Added-Mass Partitioned Algorithms for Fluid-Structure Interactions

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Key Words: fluid-structure interactions, added-mass, partitioned algorithms, overset grids

In this talk we give an overview of some fluid-structure interaction (FSI) algorithms that we have developed to solve problems with light structures where added-mass and added damping effects are large. Traditional partitioned algorithms for FSI often have difficulty for light solids and require multiple sub-iterations per time-step to remain stable. The problem is especially acute for incompressible flows and light bodies due to the effective infinite speed of sound in the incompressible fluid. The new numerical schemes we have developed, called Added-Mass Partitioned (AMP) algorithms, are partitioned algorithms that require no sub-iterations, are fully second-order accurate, and remain stable even in the presence of strong added-mass and added-damping effects. We have developed AMP algorithms for a variety of FSI regimes involving compressible and incompressible flows coupled to rigid bodies, beams and bulk solids [1, 2, 3, 4, 5]. The details of the AMP schemes differ for the different FSI regimes but a common theme is to develop novel numerical interface conditions that embed important properties of the solution. For example, for compressible fluids or solids, characteristic information is used, while for incompressible flows a balance of accelerations is enforced. These schemes have been implemented on moving and deforming overlapping grids using the Overture framework.

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Circuit-integrated fluid-structure-piezoelectricity interaction analysis for flow-driven energy harvesters

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Key Words: *Flow-Driven Energy Harvester, Partitioned iterative method, Fluid-Structure Interaction, Piezoelectricity*

The piezoelectric effect transforms electrical energy into mechanical energy and vice versa. Piezoelectric materials can thus be used to harvest energy from mechanical vibration. Flow-driven energy harvesters, which harvest energy from flow-induced vibration, have attracted attention. This type of harvester has been widely investigated in the aerospace community.

Flow-driven energy harvesting is a complex problem with coupling among the host structures, piezoelectric materials, surrounding fluid, and electric circuits. For numerical evaluation of the harvester, coupled analysis is needed. Although there have been some numerical studies on flow-driven piezoelectric energy harvesters [1], many of them introduce simplifications and detailed numerical simulations have been rarely conducted.

In our previous work, we developed FEM-based fluid-structure-piezoelectricity coupled analysis [2], where we employed a partitioned approach, which allows to use existing solvers. In the present study, we integrate circuit analysis into the coupled analysis to consider piezoelectric energy harvesters and to calculate generated energy by the harvesters. We show a two-dimensional numerical simulation on limit cycle oscillation of a cantilevered beam where piezoelectric energy harvesters are implemented. Then, the relation between the placement of the harvesters and the scavenged energy is investigated.

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Computational fluid-structure interaction with contact and turbulent flow applied to patient-specific simulation of heart valve disease

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Key Words: fluid-structure interaction, turbulent flow, patient-specific heart modelling

We present recent work on computational fluid-structure interaction with contact and turbulent flow, in the context of patient-specific simulations of the blood flow in the left ventricle of the heart. The mathematical model of the intraventricular blood flow and its interaction with the mitral and aortic valves presents challenges in terms of a complex geometry, turbulent flow, a deforming domain, and fluid-structure interaction with contact. The numerical method is based on an Arbitrary Lagrangian-Eulerian approach [1], where the blood and the valve tissues are modelled in one single computational mesh, and the implementation of the method is designed to be efficient on massively parallel computing platforms.

Such simulations have the potential to be part of the standard workflow in the clinic, for example, to support diagnosis and treatment of heart disease. Through simulation, the blood flow can be investigated in great detail and properties of the blood flow can be computed which cannot be measured by imaging techniques, such as the local blood pressure and mechanical stresses. To analyze the mechanical stresses in the blood we use the triple decomposition of the velocity gradient tensor [2], by which shear flow can be separated from straining flow and rigid body rotational flow. The level and extent of different types of mechanical stresses can lead to an elevated risk for thrombosis events. Hence, a detailed analysis of simulation data could contribute to the risk assessment of clinical interventions.

Further, the triple decomposition of the velocity gradient tensor can be used to analyze the stability of turbulent flow, hence, to characterize the smallest scales of the blood flow in the ventricle [3].

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Computational Modeling of Fluid-Structure and Contact Interaction in Large Assemblies of Highly-Flexible Fibers Immersed in Viscous Flow

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Key Words: Stokes Flow, Flexible Filaments, Large-Deformation Beam Elements, Beam Contact, Boundary Element Method, Graphic Processing Units (GPUs).

The dynamic response of flexible filaments immersed in viscous fluids is important in cell mechanics, as well as other biological and industrial processes. In this talk, we propose a parallel computational framework to simulate the fluid-structure interactions in large assemblies of highly-flexible filaments immersed in a viscous fluid. We model the deformation of each filament in 3D with a C^1 geometrically-exact large-deformation finite-element beam formulation and we describe the hydrodynamic interactions by a boundary element discretization of the Stokeslet model. We incorporate a contact algorithm that prevents fiber interpenetration and avoids previously reported numerical instabilities in the flow, thus providing the ability to describe the complex evolution of large clouds of fibers over long time spans. In order to support the required long-term integration, we use implicit integration of the solid-fluid-contact coupling. We address the challenges associated with the solution of the large and dense linear system for the hydrodynamic interactions by taking advantage of the massive parallelization offered by Graphic Processing Units (GPUs), which we test up to 1000 fibers and 45000 degrees of freedom.

We validate the framework against the well-established response of the sedimentation of a single fiber under gravity in the low to moderate flexibility range. We then reproduce previous results and provide additional insights in the large to extreme flexibility range. Finally, we apply the framework to the analysis of the sedimentation of large clouds of filaments under gravity, as a function of fiber flexibility. Owing to the long time spans afforded by our computational framework, our simulations reproduce the breakup response observed experimentally in the lower flexibility range and provide new insights into the breakup of the initial clouds in the higher flexibility range.

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Fluid–Structure Interaction Modeling for Compressible Flow Applications

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Key Words: Compressible flow, Fluid–structure interaction, Non-matching interface, Isogeometric analysis, Hybrid fluid–structure interaction, Aircraft buffeting, Arbitrary Lagrangian–Eulerian

Aircraft buffeting is an aeroelastic phenomenon characterized by random pressure oscillations impacting on the horizontal stabilizer caused due to the turbulent airflow in the wake of the wing during the different flight missions. This unsteady dynamic loads acting on the stabilizer over a longer duration can reduce its structural fatigue life. Computational modeling of aircraft buffeting has been challenging due to the aerodynamic nonlinearities and complex aircraft structural components. To numerically model and study the effects of aircraft buffeting, a high-fidelity fully-coupled compressible flow fluid–structure interaction (FSI) framework is developed in this work. The FSI methodology is developed to handle the different non-matching discretizations at the interface and a projection method is used for the transfer of kinematic and traction data between the fluid and structure subdomains. Finite element based Navier–Stokes equation of compressible flow and the isogeometric analysis (IGA) based rotation-free Kirchhoff–Love shell structural formulation are considered to model the physics involved. The method is validated for its accuracy through a benchmark problem and is applied to simulate flow around full-scale aircraft and the buffeting of its horizontal stabilizer. A novel hybrid FSI methodology is also developed specifically in the application to model aircraft buffeting. The FSI framework is also extended to model the aircraft maneuvers based on arbitrary Lagrangian–Eulerian (ALE) approach to simulate realistic time-dependent flight paths and study the effects of unsteady loads acting on the horizontal stabilizer of the aircraft.

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Integrated Modeling of the Human Left Heart: Coupling Electrophysiology, Mechanics and Fluid Dynamics

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Key Words: Cardiac modeling, Electrophysiology, Fluid-structure interaction, Multiphysics

We propose an integrated computational model of the human heart [1], comprising three-dimensional descriptions of electrophysiology, active and passive mechanics and hemodynamics, resulting in an electrophysiology-fluid-structure interaction bidirectionally coupled model. We incorporate the effect of external circulation with a lumped parameters model [3]. We explicitly describe the interplay between the different phenomena occurring within the heart. We rely on the monodomain equation for cardiac electrophysiology. Muscular activation is described with the model presented in [2]. Passive mechanics is modeled in the hyperelastic framework using Guccione and Neo-Hooke models [3]. We use incompressible Navier-Stokes equations in ALE framework for blood dynamics, with the RIIS method for of valves [4]. We rely on a staggered scheme for time discretization. All coupling terms are treated explicitly, but for fluid-structure coupling, treated implicitly with a monolithic approach [5]. We discretize in space with the finite element method. Simulations on a realistic human left heart showcase the ability of our model to reproduce physiological behavior. This project has received funding from the ERC under the European Union's Horizon 2020 research and innovation programme (grant agreement No 740132, iHEART - An Integrated Heart Model for the simulation of the cardiac function, P.I. Prof. A. Quarteroni).

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Separation Simulation and Compatibility analysis of multibody aircraft with consideration of aeroelasticity

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Key Words: *Multibody Aircraft, Separation, Compatibility, Aeroelasticity*

Multi body aircraft can significantly improve the dynamic and tactical characteristics of aircraft by the combining and separating of multi-body structure. This concept has been applied to ammunition and carrier rockets maturely and with promising benefits for application of cluster unmanned aerial vehicles (UAV) and reusable launch vehicles (RLV). Different from the conventional aircraft, multi-body aircraft no longer restrict and contact each other after separation. The interference effect of flow field in separation process will lead to significant nonlinearity in aerodynamic and separation dynamic characteristics. With the improvement of flexibility and layout complexity of modern aircraft, additional aerodynamic force caused by elastic deformation in the separation process can no longer be ignored, which further complicates the separation system[1-5]. For analysing the influence of aeroelastic effect on separation process of multi-body aircraft, a shrapnel-like aircraft is selected as an example, the time-domain fluid-structure interaction (FSI) method based on overset grid is adopted and separation process of multi-body aircraft system at different initial angle of attack (AOA) is analyzed in this paper. Where separation compatibility under different relative position conditions is divided into safety and effectiveness, which is discussed respectively and compared with simulation results based on rigid body dynamics. The results show that the deformation of structure is dominated by low-order bending modes under the consideration of aeroelastic effect. As time marching, the influence of elastic deformation on the trajectory develops incrementally, which has an influence on separation compatibility, which cannot be ignored. Influence caused by AOA of carrier craft on the sub-craft trajectory changes monotonously along the z-axis direction, while influence caused by AOA of sub-craft on the compatibility tends to be consistent. The work of this paper will provide a reference for the design and control of cluster like multi-body aircraft.

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Space–Time Computational Methods for a Tsunami-Shelter Vertical-Axis Wind Turbine

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Key Words: Vertical-axis wind turbine, Tsunami shelter, Space–Time Variational Multiscale method, ST Isogeometric Analysis, NURBS mesh generation

We present space–time (ST) computational methods and flow analysis for a vertical-axis wind turbine (VAWT) that has been proposed to also serve as a tsunami shelter. Much of this research has been reported in [1]. In this presentation, we focus on the computational methods. Computational challenges encountered in flow analysis of wind turbines in general include accurate representation of the turbine geometry, multiscale unsteady flow, and moving-boundary flow associated with the rotor motion. The tsunami-shelter VAWT, because of its rather high geometric complexity, poses the additional challenge of reaching high accuracy in turbine-geometry representation and flow solution when the geometry is so complex. We address the challenges with an ST computational method that integrates three special ST methods around the core, ST Variational Multiscale (ST-VMS) method, and mesh generation [2] and improvement methods [3]. The three special methods are the ST Slip Interface (ST-SI) method, ST Isogeometric Analysis (ST-IGA), and the ST/NURBS Mesh Update Method (STNMUM). We present computations for the 2D and 3D cases. The computations show the effectiveness of our ST and mesh generation and relaxation methods in flow analysis of the tsunami-shelter VAWT.

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Time-splitting Schemes for Fluid–Structure Interaction in Biomedical Applications

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Key Words: Fluid–structure interaction, split-step scheme, semi-implicit coupling, hemodynamics, incompressible flow, non-Newtonian fluid

The interaction of incompressible flows and elastic structures plays a central role in numerous applications in biomedical and general engineering and has thus been a very active area of research during the recent years. Advances in the field have enabled patient-specific fluid–structure interaction (FSI) simulations in the cardiovascular and respiratory context, greatly increasing the impact of numerical tools on diagnostics, treatment, device design and deployment. However, the ever increasing model complexity and high computational demand still pose great challenges even to modern supercomputers.
In this context, we present a partitioned FSI algorithm involving incompressible flows of non-Newtonian fluids and three-dimensional continua [1]. Fluid velocity and pressure are decoupled using a pressure Poisson equation and extrapolation in time, leading to an iteration-free time-splitting (or split-step) scheme allowing for equal-order interpolation, which was originally developed for flows of non-Newtonian fluids on fixed grids [2]. Similar to [3], this setup allows for added-mass stable semi-implicit FSI, merely coupling fluid pressure and structure displacement iteratively. To further boost performance, we enforce Robin interface conditions and apply an interface quasi-Newton method [4].
The framework is showcased considering the blood flow through a patient-specific geometry of an iliac bifurcation and an idealised setup of human phonation, both using parameters in the physiologically relevant range.

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Ventricle-Valve-Aorta Flow Analysis with the Space–Time Isogeometric Discretization and Topology Change

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Key Words: Ventricle, Heart valve, Aorta, Medical image, Space–time method, Isogeometric discretization, Inflow stabilization, T-spline discretization

We address the computational challenges of and present results from ventricle-valve-aorta flow analysis. Including the left ventricle (LV) in the model makes the flow into the valve, and consequently the flow into the aorta, anatomically more realistic. The challenges include accurate representation of the boundary layers near moving solid surfaces even when the valve leaflets come into contact, computation with high geometric complexity, anatomically realistic representation of the LV motion, and flow stability at the inflow boundary, which has a traction condition. Much of this research has been reported in [1]. The challenges are mainly addressed with the space–time (ST) computational method "ST-SI-TC-IGA" [2]. The ST-SI-TC-IGA integrates three special ST methods around the core, ST Variational Multiscale (ST-VMS) method [3]. The three special methods are the ST Slip Interface (ST-SI) [4] and ST Topology Change (ST-TC) [5] methods and the ST Isogeometric Analysis (ST-IGA) [3]. The Constrained-Flow-Profile Traction [1], as a special method, provides flow stability at the inflow boundary. The computation with the LV-valve-aorta model shows the effectiveness of the ST-SI-TC-IGA.

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Ditching Simulation of Aircraft. A Comparative Analysis of Different Computational Approaches.

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Key Words: *Ditching, Computation, Fluid-Structure Interaction, Flexible structure*

Novel aircraft designs must be compliant to crashworthiness certification requirements. One requirement is to investigate the behaviour of the aircraft exposed to the hydrodynamic loads expected in a planned emergency landing on the water, commonly known as ditching. Contrary to an unexpected and unprepared crash on water, ditching is characterized by the level of preparation prior to the impact. Low approach speeds, a nose-up position of the aircraft, the consideration of the sea state and the direction of the wind as well as the cabin preparation are pursued by the pilots and the crew in order to reduce the impact loads and decelerations to increase the survivability of the occupants and to allow their subsequent evacuation [1].

Aircraft manufacturers can apply diverse methods to demonstrate compliance with respect to ditching requirements. Nevertheless, computational numerical approaches in combination with detailed aircraft models allow for the analysis of the global kinematics of the aircraft, and for the investigation of the local airframe structural integrity. The numerical simulation of ditching is very challenging, because the fluid moves at considerably high velocity and the structure undergoes large nonlinear deformations due to high hydrodynamic loads. For this kind of coupled analysis, different numerical methods were investigated; mainly mesh free Lagrangian methods such as the coupled Finite Element-Smoothed Particle Hydrodynamics on one hand or the Arbitrary Lagrangian Eulerian methods [2]. The coupling between the fluid modelled with SPH and the structure is based on a node to surface contact interface, while the Coupled Euler-Lagrange computational approach uses an embedded contact interface between the fluid (ALE formulation) and the structure. A flexible reinforced bottom-aircraft panel made of a skin, frames and stringers in aluminium alloy and modelled with bi-linear quadrangular shell elements under guided ditching conditions was considered in previous work [3]. Detailed results obtained for the different computational approaches are compared here in terms of global and local time histories.

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Comparison of Actuator-Disk Based LES and RANSE Predictions in Farm Flow Simulations

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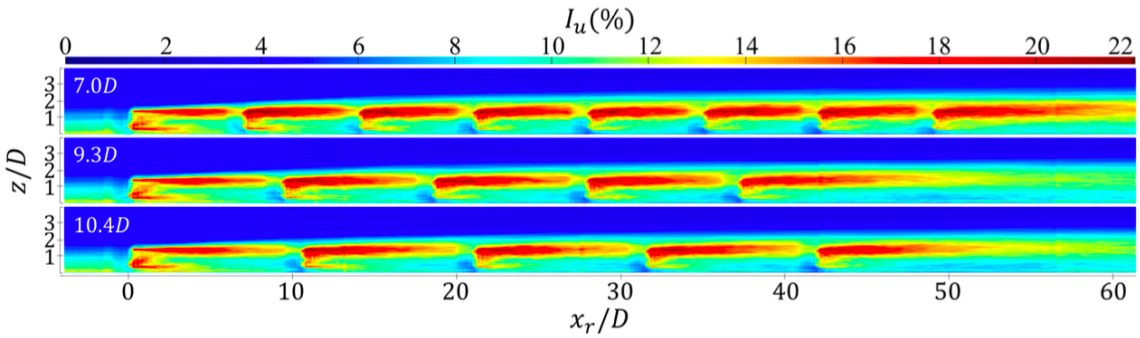
Key Words: *LES, RANSE, Actuator Disk, Wind Farm, Wake*

The wind farm flow simulations are compared between RANSE and LES predictions in this paper, where an actuator disk model is employed in describing the interactions between the incoming airflow and the wind turbine rotor.

This paper proposes a simplified nonlinear wake model that fills the technical gap between the low-cost and less-accurate linear formulation and the high-cost and high-accuracy large eddy simulation, to offer a suitable balance between the prediction accuracy and the computational cost, and also to establish a robust approach for long-term wind farm power prediction. A simplified actuator disk model based on the momentum theory is proposed to predict the wake interaction among wind turbines along with their power output. The three-dimensional flow field of a wind farm is described by the steady continuity and momentum equation coupled with a k-ε turbulence model, where the body force representing the aerodynamic impact of the rotor blade on the airflow is uniformly distributed in the Cartesian cells within the actuator disk.

This paper also develops a large eddy simulation (LES) approach to predict wind farm flows. The standard Smagorinsky model with Mason damping function is used for modeling the subgrid-scale stress. The governing equation is discretized by a finite volume method, where a SIMPLE algorithm is adopted. The bounded-central differencing scheme with a hyper-tangent blending function is proposed in the convection term approximation. An actuator disk method is employed to model the impact of rotor on the incoming airflow. A synthetic inflow formulation is applied to simplify the specification of the inflow boundary condition. The proposed LES framework is implemented in an in-house code, WIFA3D-LES.

The Horns Rev wind farm is selected as the target site to examine the wind farm flow characteristics predicted by both approaches.



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Enhanced vortex-induced vibration of two side-by-side circular cylinders at Re = 1000

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Key Words: vortex-induced vibration, VIVACE, side-by-side, direct-forcing immersed boundary

Vortex-induced vibration (VIV) of bluff bodies such as a circular cylinder is one of the most attractive fluid-structure interaction (FSI) topics. When dealing with the multiple cylinders, the VIV responses for both cylinders are relatively complex. Recently, a number of studies have focused on enhancing the VIV phenomena for energy harvesting devices such as VIVACE (Vortex-Induced Vibration for Aquatic Clean Energy). In the present work, three-dimensional numerical simulations of two side-by-side vibrating cylinders are performed at Re = 1000. This study has been performed using a direct-forcing immersed boundary (DFIB) method. The numerical simulations are conducted in the range of reduced velocity $2 < U_R^* < 10$. The vibration responses of the two cylinders are studied for a range of gap ratios $1 < g^* < 3$. In addition, the fixed circular cylinder is placed in front of the vibrating cylinder to enhance VIV responses.

It was found that the side-by-side cylinders with $g^* = 1 - 1.2$ produce a higher vibration amplitude much larger than the response of a single cylinder in the initial excitation region. In the lock-in region, almost all side-by-side cylinders produce smaller vibration amplitudes than the single-cylinder response. A fixed circular cylinder in front of the vibrating cylinder increases the vibration amplitude in the lock-in and desynchronization regions without changing or shifting the lock-in frequency range. The wake interaction from the fixed cylinder in front of the vibrating cylinder produce this enhanced VIV response.

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Flow Analysis for Bionic Shark Denticle Structure by the Variational Multiscale Finite Element Method

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Key Words: *Finite Element Method, Incompressible Navier Stokes Equation, Shark Denticle, Variational Multiscale Large Eddy Simulation.*

The unique geometry of the microstructure on the shark-skin surface, known as denticles, is the main reason sharks can swim at high speed [1]. In order to discover the relationship between the complicated denticle structures with the associated flow pattern, we perform a series parameters study, including the drag force analysis and flow stability study under different denticle geometry. In this research, the incompressible Navier Stokes (N-S) equation is chosen as the fluid model; the Galerkin finite element method with variational multiscale method (VMS) [2][3] is adapted. The VMS aims to stabilize the instability due to the advection in the N-S equation, as well as introduces the fine-scale terms that act as the large eddy simulation (LES) in the fluid model. The framework was implemented under the open-source finite element platform, called FEniCS [4]. We first perform the numerical testing on the flow over a sphere and a bionic shark-skin structure to investigate the flow pattern under different Reynolds number, which validates the effectiveness of the proposed framework. Then, a parameter study is employed for different shark species with associated unique shark denticle geometry. The drag-reduction effects among different shark-skin are revealed, and can be used as a reference for future design on the bio-inspired structure.

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Fluid-structure interaction simulations using immersed boundary method and general pressure equation

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Key Words: General pressure equation, Immersed boundary method, fluid-structure interaction

The general pressure equation-based method[1] is fully explicit, and the method does not require either solving the pressure Poisson equation nor executing sub-iteration for incompressible flow simulation. However, few numerical validations of general pressure equation method are available, especially under complex flows like fluid-structure. In this work, general pressure equation based method is used to conduct numerical simulations of flows with embedded solid object modeled by the immersed boundary method[2, 3, 4, 5]. Several fluid-structure interaction test problems are used to demonstrate the capability of the current approach. The simulations are conducted on GPU cluster using MPI and CUDA[1, 6].

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Numerical simulations of dynamic stall of airfoil under plasma control in turbulent flow

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Key Words: Flow Control, Plasma Actuator, Dielectric Barrier Discharge, Vortex Generator, Computational Fluid Dynamics

Abstract: An airfoil is a shaped surface that produces lift and drag when moving through the air, such as an airplane wing, tail, or propeller blade. Stall is a physical phenomena in which lift falls quickly due to a large angle of attack (AOA) surpassing the critical value. The fundamental reason for this is that the boundary layer flow above the airfoil separates early, resulting in vortices in the separated flow that account for the majority of the top airfoil surface. Dynamic stall is a complex fluid dynamics problem that occurs on an airfoil when the angle of attack exceeds the static stall limit during rapid, transient motion. In this study, a dielectric barrier discharge (DBD) plasma actuator was used to control the dynamic stall of an oscillating NACA0012 airfoil. In the current study, the following four cases were investigated based on different frequency of DBD : **(A)** 2KHz, **(B)** 3KHz, **(C)** 4KHz, and **(D)** 6KHz. Overall, instantaneous results and supplementary movies have been provided to demonstrate the effect of DBD to help better understand vortex patterns affected by different plasma parameters. The line plasma DBD can improve the lift-drag coefficient ratio of an airfoil during pitching since it can reduce drag during upstroke and downstroke. In terms of numerical results, it is recommended that using high-frequency increases the lift-drag ratio and delays stall in the complete stroke.

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SUPPLEMENTARY MOVIES:

Supplementary movies are available at https://youtu.be/C87Ji2b0z8I.

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Numerical Study of Superbike Aerodynamic Wing Kit Configurations Using k-ω SST Turbulence Model

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Key Words: *k-ω SST turbulence model, OpenFOAM, NACA 4412, aerodynamic wing kits*

In the past few years, the use of computational fluid dynamics (CFD) to increase downforce on superbikes has been a part of the winning strategy for racing teams. This study aims to find the highest lift-to-drag (L/D) ratio for aerodynamic wing kit configurations with various angles of attack (AoAs) and wind speeds. Based on the SIMPLE algorithm, the k-ω SST turbulence model has been chosen to solve Reynolds-averaged Navier–Stokes equations using OpenFOAM CFD software. All cases using NACA 4412 as the basic airfoil with a wingspan of 0.6 m are able to comply with the technical regulations revised by the Fédération Internationale de Motocyclisme (FIM). The benchmark validation is based on numerical comparison between OpenFOAM and JavaFoil software. Case 0 contains a partial fairing with a wing for grid independence study. The converged results of the near-wall y-plus in the range 0.01 to 2 have been applied to the rest simulations to improve the accuracy of viscous sublayer. Case 1 contains a complete superbike with wings and a rider. According to the results of Case 1, Case 2 uses the highest L/D ratio of -37 degrees as the upper fixed-wing and adds another lower wing placed at an appropriate position. In Case 3, we replaced non-parallel wings with parallel wings. Case 4 uses the highest L/D ratio above all cases, and modifies the 3D model by using a closed wing and obtains L/D ratios in accordance with the FIM regulations. In conclusion, in Case 3, the AOA of -41 degrees parallel wings has the highest L/D ratio. Based on the results, the L/D ratio in Case 4 is -0.2, and the lift coefficient is -0.06. Compared with the lower wing, the upper wing provides higher downforce. Further study aims to visualize the vortex generation using various vertical wing struts based on Case 4. Subsequently, the popularization of aerodynamic wing kits will contribute to the safety of superbike driving.

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Numerical study of Savonius wind turbine using direct-forcing immersed boundary method

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Key Words: *Savonius wind turbines*, *aerodynamic performance, tip speed ratio, direct-forcing immersed boundary model*

There are two methods for accounting for rotor rotation in the computational domain of a fluid flow equations when conducting numerical simulations to predict the aerodynamic performance of Savonius wind turbines: rotor with constant angular velocity and rotor in an inertial reference frame with variable rotor angular velocity [1,2]. So far, a number of numerical studies have been carried out to investigate the performance of the Savonius rotor using a constant angular velocity approach. However, there is a lack of detailed descriptions about the systematic investigation of azimuthal increments per time step and the number of turbine revolutions impact on the accuracy of CFD simulations results at different tip speed ratios. The purpose of this study is to simulate a three-dimensional model of a Savonius rotor in order to evaluate its aerodynamic performance and to investigate computational parameters such as azimuthal increment and the number of turbine revolutions effect on the accuracy of simulation results at different tip speed ratios. The prominent performance parameters such as instantaneous dynamic torque coefficient (C_t) and power coefficient (C_P), were investigated for each case using a direct-forcing immersed boundary (DFIB) numerical model. A few azimuthal increment angles are investigated and the best value is selected. Furthermore, the steadiness of simulation results is determined in relation the number of turbine rotations. The study found that the azimuthal increment per time step is highly dependent on the tip speed ratio. The present results provide insight into the systematic relationship between azimuthal increments and the number of turbine revolutions on the accuracy of the Savonius rotor simulation results at different tip speed ratios.

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Force Performance and Vortex Structure of Flapping Foil in Unsteady Ground Effect at Moderate Reynolds Number

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Key Words: flow-structure interaction, flapping foil, ground effect

In this presentation, a symmetrical foil with combined heaving-and-pitching motion in the unsteady ground effect, that is, close to a solid boundary, at moderate Reynolds number is numerically investigated with varying flapping frequency, f, but fixed amplitude. It is naturally expected that the distance between the foil pitching axis and the ground, d, would make a significant influence on the force performance and vortex structure on flapping foil, compared with that in unbounded freestream[1]. To quantitatively evaluate the effect of d, an acceleration-based velocity corrected immersed boundary method [2] is adopted after being validated with previous experimental and numerical results in literature. With the assistance of numerical simulation, we find that the time-averaged force in streamwise direction increases monotonically as the distance between foil pitching axis and ground decreases. Meanwhile, with decreasing distance d, the time-averaged force in transverse direction changes from a lift force to a suction force, causing a equilibrium altitude[3]. The time evolution of force in transverse direction shows a sudden decrease due to the blockage effect and recirculation. By varying the Reynolds number from 1000, which is large enough making the viscous effect negligible[4], to 50, the force performance is deteriorated with increasing viscosity due to the interaction between trailing edge vortex and boundary layer vortex.

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Reducing velocity error and its consequences by an iterative feedback immersed boundary method

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Key Words: Immersed boundary method, Boundary velocity error, Streamline penetration, Blood flow

The immersed boundary method (IBM) has attracted growing interest in the computational fluid dynamics (CFD) research community due to its simplicity in dealing with moving boundaries in fluid-structure interaction (FSI) systems [1]. We present a study on streamline penetration, velocity error and consequences of a FSI solver based on an iterative feedback IBM. In the FSI, the fluid flows are solved by the lattice Boltzmann method; the solid structure deformation is solved by the finite difference method, and an iterative feedback IBM is used to realize the interaction between fluid and structure. The iteration can improve the no-slip and no-penetration boundary conditions at the fluid-solid interface. Four benchmark cases are simulated to study the reduced velocity error and its consequences: a uniform flow over a flapping foil, flow-induced vibration of a flexible plate attached behind a stationary cylinder in a channel, flow through a two-dimensional asymmetric stenosis and a one-sided collapsible channel. Results show that the iterative IBM can suppress the boundary-slip error and spurious flow penetration on the solid wall. While the iterative IBM does not have significant effect on the force production and structure deformation for external flows, it significantly improves the prediction of the force distribution and structure deformation for internal flows. The increased computational cost incurred by the iteration can be largely reduced by increasing the feedback coefficient. This study will provide a better understanding of the feedback IBM and a better option for the CFD community.

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VALIDATIONS OF A WALL MODEL IN THE IMMERSED BOUNDARY--LATTICE BOLTZMANN METHOD

TRACK NUMBER (--)

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Key words: Immersed Boundary—lattice Boltzmann method, wall modelled large eddy simulation and fluid—structure interaction.

ABSTRACT

The wall modelled large eddy simulation (WMLES) in the immersed boundary--lattice Boltzmann method (IB—LBM) is examined by considering two benchmark validations, i.e., flow around a hull of submarine and cylinder. Specifically, the diffusive wall model proposed by Shi et al. is incorporated into the IB—LBM solver to model the high Reynolds number turbulent flow. To maintain the numerical stability, two collision models, i.e., multiple-relaxation-time (MRT) and recursive regularized (RR), are implemented. The performance of these models in the WMLES is examined and compared by considering both the prediction of aerodynamic force and flow fields. It is found that diffusive wall model is capable to achieve excellent results for turbulent flow modelling involving fluid—structure interaction. The two collision models give close results for the aerodynamic force, but the MRT collision model shows spurious non-physical oscillations in the flow field, making the RR collision model a better choice for the high Reynolds number turbulent flow modelling.

Wall Model-Based Diffuse-Interface Immersed Boundary Method for Simulation of Incompressible Turbulent Flows

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Key Words: *Immersed boundary method, Diffuse-interface, Wall model, Turbulent flow*

In this work, a method is proposed to simulate the high Reynolds number turbulent flows by combining the diffuse-interface immersed boundary method (IBM) with two wall models. In this method, two auxiliary layers (a series of Lagrangian points) are set outside the wall: the reference layer and the enforced layer. The wall model is applied at the reference layer to calculate the wall shear stress and the boundary condition is implemented at the enforced layer. When implementing the boundary condition, the implicit velocity correction-based IBM is used. This process requires the velocity at the enforced layer. To calculate the velocity at the enforced layer, the momentum equation is integrated along the normal direction of the wall to link the tangential component of the velocity to the wall shear stress predicted by the wall model, and the normal component of the velocity is approximately reconstructed by the parabolic distribution. In addition, Reichardt's law combined with Spalding's formula is utilized to determine the integral length. In this method, the distances between the two auxiliary layers and the wall (Δ_F and Δ_1) are two very important parameters, and Δ_1 further determines the value of the integral length Δ_P. Numerical results show that these two parameters will greatly affect the results and their values should be preferably changed together with the thickness of the boundary layer. Overall, the locations of auxiliary layers are affected by the grid size and the Reynolds number, and they should be as close as possible to the wall. But, due to the limitation of the influence range of the Dirac delta function, which will interfere with the calculation, the distance between the two auxiliary layers should not be too small. This is to avoid the overlapping of the interpolation range between the Lagrangian points of the two auxiliary layers. So how to resolve the contradiction between the limitation of the influence range of the interpolation function and the thin thickness of the boundary layer close to the leading edge still needs further study.

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Acoustic-Structure Coupling Modeling and Dynamic Analysis of Pump-pipeline System

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Key Words: *Acoustic-structure coupling, Pump-pipeline System, Pressure Fluctuation, FEM Dynamic Model*

The coupling effects of the acoustic and structure on dynamic response of the petrochemical pump-pipeline system are investigated by the dynamic modeling and numerical analysis. An actual equipment that consists of two centrifugal pumps, two valves and spatially arranged pipes is aimed to build its FEM dynamic model with the acoustic-structure coupling effect. The FEM modeling involves shell finite element for the structure and 3-D acoustics element for the sound field inside the pipes and the pumps. The vibration characteristics of the pump-pipeline system, including modal and amplitude frequency response, are obtained from the numerical analysis. The numerical results are in good agreement with actual test data, thus validating the presented model. It is found that the dynamic response of the pump-pipeline system under different influence factors are substantially different. The pressure fluctuation of pump fluid possess the significantly interactional influences on the dynamic characteristics of the pipe. Small pressure fluctuation could impact the acoustic-structure coupling system, resulting in remarkable changes in the dynamic characteristics of the pipeline. The effects of sound velocity and the density of fluid on structural dynamic behaviours and the corresponding mechanism are discussed.

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Dynamic Mode Decomposition of Lead-Bismuth Eutectic Turbulent Flow in a Wire-Wrapped Single Rod Channel

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Key Words: *Dynamic Mode Decompostion, Wire-Wrapped Rod Fuel, Lead-Bismuth Eutectic, URANS*

Lead-Bismuth Eutectic (LBE) alloy has been used as coolant for next generation liquid metal fast reactor. The thermal-hydraulics as well as flow-induced vibration of wire-wrapped rod bundles are primary concerns for fast reactor safety design. This calls for accurate and fast fluid field simulation and prediction for wire-wrapped rod fuel assembly, yet it remains a challenge due to the complex geometries and high Renolds number flow in wire-wrapped rod channel. This work presents a data-driven dynamic mode decomposition (DMD) method applied to the turbulent flow in a single wire-wrapped rod channel. The time-series data of fluid velocity and pressure were modelled and collected by using URANS turbulence model. Model analysis was performed over the snapshot matrix and DMD modes were obtained. The DMD modes were then used to construct a reduced-order system for fast fluid field reconstruction and forecasting. The correctness and feasibility of the method was demonstrated and compared with ground truth CFD simulation results. Our method offers a fast and reliable approach for reduced-order modelling of turbulent flow in wire-wrapped rod fuel assemblies.

Study on the behavior of bubbles colliding with hydrophilic and hydrophobic curved walls

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Key Words:*Bubble; Wettability; Collision; Liquid film drainage*

The research on the behavior and influencing factors of bubble collision has always been one of the focuses of scientific research. Its application in industrial fields such as mineral flotation and gas film drag reduction is of great scientific value. This work focuses on the effect of curved wall on bubble impact behavior. The impact process of bubbles colliding with hydrophilic and hydrophobic curved wall under different radius of curvature was measured by high-speed camera technology, and the effects of wettability and radius of curvature on bubbles colliding with solid curved wall were analyzed. The results show that when the bubble collides with the hydrophilic curved wall, it will bounce many times until it leaves the curved wall; The larger the radius of curvature is, the less the number of jumps will be. In addition, a theoretical model is established to predict the liquid film drying time, which is mainly related to the initial distance, curved wall curvature radius, bubble diameter, liquid viscosity and critical fracture thickness. The prediction error is less than 5.0%. The prediction results accord with the experimental results. This model can be used to predict and analyze the drainage time of bubble impacting hydrophobic curved wall liquid film, so as to provide a certain theoretical basis for related projects.

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Underwater Explosion (UNDEX) and Air-Blast Fluid Structure Interaction using Penalty and Strongly coupled Immersed-IGA-Peridynamics

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Key Words: Underwater Explosions (UNDEX), Fluid-Structure Interaction (FSI), Isogeometric Analysis (IGA), Peridynamics, Computational Fluid Dynamics (CFD), Composites

Blast loading of structures continues to pose challenges with respect to the resolution of fluid and structural response, especially in 3D. Additionally, the naval industry has specific interest in problems involving underwater blast-structure interaction. Shallow underwater blasts from explosive charges result in a high pressure gas region expanding into ambient pressure water and a resulting shock which propagates in the immersing fluid. This bubble collapses due to momentum driven overexpansion. Cavitation in water also influences structural response in water compared to other fluids. Air and underwater blast subject immersed structres to extreme loading, resulting in complex deformation and damage behavior. A new coupled immersed-IGA-peridynamic framework is used to addresss these challenges.

In this work, the performance of an air-blast immersed-isogeometric-peridynamic density primitive reduced-energy formulation is studied in three dimensions and subsequently modified for the computation of underwater blast phenomena. Initialized domains consisting of fluid materials satisfying both the ideal gas equation of state in the air-blast case and Jones-Wilkens-Lee (JWL) equations of state in the underwater blast case in a density primitive reduced-energy compressible flow formulation are evolved using an immersed method. Solid materials are introduced as immersed particle solids, and explosive charges are introduced as immersed particle fluids. The focus of this study is on the detonation of Trinitrotoluene (TNT) in air and 1,3,5-Trinitro-1,3,5-triazinane (RDX) in water. Improvements in artificial viscosity discontinuity capturing tailored for JWL materials and ideal gas are shown to effectively stabilize the formulation.

Fluid (background and foreground) is coupled to peridynamic solids using a strong coupling as well as a penalty based approach. Penalty based coupling shows significant improvement in the deformation in coupled solid materials. In the interest of efficiency in 3D, scenarios which involve thin structures use Elastic and Kirchoff-Love shell formulations for solids. This framework couples code built on PetIGA and Petsc to modified versions of Peridigm. Additionally, a microplane concrete model is implemented in Peridigm for use in the air-blast study.

Expansion of explosive gas products results in under-integration as particles spread. Long-time stability of immersed detonation charges is aided through mass-preserving quadrature volume update on all im-

mersed fluid domains, naturally implemented in the density primitive formulation. This development is coupled with artificial viscosity based discontinuity capturing as well as JWL specific discontinuity capturing to form a robust framework for air and underwater blast structure computations. One dimensional water shocks and underwater detonations are demonstrated to agree with benchmark results. A collection of underwater 1D and 3D examples are provided to illustrate the performance of the new methodology.

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A Hybrid Continuum–Discrete Method for Numerical Simulation of Granular Impact Dynamics

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Key Words: *Granular Impact, Solid–granular Interaction, Continuum–discrete Coupling*

Granular impact – the dynamic intrusion of solid objects into the granular material – is a common phenomenon in many geotechnical engineering problems, such as dynamic compaction and rockfall protection. Still, however, it remains a significant challenge to efficiently simulate the granular impact dynamics as it involves rapid and complex interactions between the intruder and grains. So far, these intruder–grain interactions have been modeled by either a purely discrete (e.g. [1]) or a purely continuum method (e.g. [2]). However, their computational efficiency is sub-optimal due to the grain-by-grain representation of granular materials in a purely discrete method, or an extremely small time-step restricted by the high stiffness of the intruder in a purely continuum method. In this presentation, we introduce a hybrid continuum-discrete method which seeks to strike the balance between discrete and continuum methods for granular impact dynamics. Our method couples the material point method (MPM), which can efficiently simulate granular materials as continua, and the discrete element method (DEM), which can efficiently model the solid intruder as a rigid body. The method is validated by simulating laboratory test of a solid sphere dropped onto loose dry sand. Through a number of parameter studies, we also identify key factors for successful simulations of granular impact dynamics using the hybrid continuum–discrete method.

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A New Assumed Deformation Gradient Approach to Mitigating Volumetric Locking in Explicit Material Point Methods

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Key Words: Material Point Methods, Volumetric Locking, Assumed Deformation Gradient

The material point method (MPM) is commonly used to simulate large deformations in various types of nearly incompressible materials such as water and undrained soils. When applied to nearly incompressible materials, however, standard MPM schemes suffer from volumetric locking – overly stiff behavior accompanied with erroneous strain and stress fields – due to their use of low-order basis functions and many integration points. To date, several classes of approaches have been put forward to address volumetric locking in MPM. However, the existing approaches require significant modifications of the basis functions, governing equation, or the time-integration scheme, making it onerous to apply them to standard explicit MPM schemes. In this talk, we present a new approach to mitigating volumetric locking in MPM, which features an unprecedented combination of simplicity, efficacy, and generality for a class of standard explicit MPM schemes. The key idea is to combine the assumed deformation gradient ($\bar{\boldsymbol{F}}$) method [1], which was originally developed for finite element methods, with a standard projection operation in MPM. The approach has two significant advantages: (i) it does not require any modification of the existing basis functions, governing equation, or the time-integration scheme, and (ii) it can be applied to any types of nearly incompressible materials. Numerical examples will demonstrate that the new approach is effective for two popular MPM interpolation schemes – the generalized interpolation material point (GIMP) and B-spline methods – and for various types of nearly incompressible materials including a Newtonian fluid, hyperelastic solid, and an elasto-plastic solid.

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A Two-dimensional Bio-chemo-hydro-mechanical Model for In-situ Stabilization of Soils using Biochemical Processes

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Key Words: *MICP, Galerkin Finite Element Method, BCHM model, Return Mapping Algorithm*

Ground improvement techniques involving chemical additives are often energy-intensive and unsustainable due to the environmental distress caused by them. Sustainable biocementation processes such as microbially induced calcite precipitation (MICP) can overcome the drawbacks of traditional ground improvement techniques[1]. Capturing the underlying coupled mechanisms in the biocementation process requires the knowledge of diverse fields of bio-chemo-hydro-mechanics. Modeling such a complex phenomenon is imperative for the successful implementation of the stabilization technique in the field. The existing coupled models on biocementation are chiefly intended to validate the observed behavior of laboratory-scale biocemented specimens[1]. This scenario demands the need to develop a coupled bio-chemo-hydro-mechanical (BCHM) model for field simulations. The BCHM model was developed with finite element and backward Euler finite difference approximations in space and time. The Galerkin weak formulations are derived for the mass balance equations of the coupled model. The advective-governed transport phenomena are accommodated with the Petrov-Galerkin formulation. An overall kinetically controlled reactive model is implemented to reproduce the urea hydrolysis and associated chemical kinetics[1]. The reduced permeability of the biocemented soil is accounted in terms of its effective porosity, using the modified Kozney-Carman equation[2]. The fixed point iteration method is implemented for bio-chemo-hydraulics to deal with the nonlinearity in the balance equations. The mechanical constitutive response of biocemented soil is simulated using a micromechanical framework. The von Mises and Drucker-Prager plasticity models were adopted for the biocement and soil particle phases, respectively[3]. The integration of plasticity models was carried out using a return mapping algorithm[3]. The Newton Raphson scheme is considered for the finite element implementation of elastoplastic models. The fully coupled nonlinear finite element problem is solved in a staggered approach using the developed MATLAB routine. The contour plots of biomass and chemical concentrations and precipitated calcite content are generated. The iso error maps are acquired for the inspection of the error behavior of the integration algorithm. The considered elastoplastic models predicted improvement in mechanical strength of biocemented specimen. A complete bio-chemo-hydro-mechanical behavior of the two-dimensional geometry is captured.

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Hyperelastic Model for Geomaterials: Its Significance in Coupling with Plasticity for Finite Strain

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Key Words: *Geomaterials, Hyperelasticity, Cam-clay plasticity, Anisotropy, Finite strain*

This study is aimed at developing a formulation of hyperelastic model for geomaterials and combining it with plasticity. Several existing representative isotropic hyperelastic models with pressure-dependent bulk and shear moduli are reformulated to extend them to finite strains [1–4]. To be compatible with the framework of multiplicative finite strain elastoplasticity, the stress versus the elastic strain relation, together with the fourth-order elastic tangent moduli tensor, in the description relative to the intermediate configuration is derived for each of the hyperelastic models. Their spatial and material descriptions are also derived. A systematic parametric study with a particular focus on the pressure-dependent property of the elastic moduli is performed to examine and compare the constitutive response of the hyperelastic models under typical cases of simple shear and triaxial compression. Significant differences in the hyperelastic responses depending on the types of model are observed in the analysis. Notably, some models exhibit unexpected unreasonable decrease in stress in the process of triaxial compression.

The hyperelastic models are then combined with plasticity. The Cam-clay plasticity with rotational hardening is adopted as a specific prototype model for geomaterials exhibiting induced anisotropy. A formulation of the elastoplastic model based on the multiplicative framework, as well as a stress-point algorithm using fully implicit return-mapping scheme, is developed [5]. Numerical examples are presented to demonstrate the significance of hyperelastic model in the analysis of elastoplasticity. The analysis result reveals that the property of hyperelastic model has significant influences not only in the responses of elastoplastic model but also in the computational aspect to ensure stable analysis.

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Multiphysics finite element analysis of intermediate-depth earthquakes

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Key Words: *intermediate-depth earthquakes, extended finite element analysis, phase transformation, thermo-mechanical*

While less common and less studied than shallow earthquakes, intermediate-depth earthquakes comprise around 90% of deep earthquakes and cause significant damage and casualties. Defined here as earthquakes that occur between 50-350 km depth, the mechanisms that drive them are still not completely understood. Extreme pressures preclude the frictional sliding that dominates shallower events, and low void ratios suggest that fluid pressure probably does not play a major role. Because these events cannot be observed directly, a combination of small-scale experiments, numerical modelling, and seismological data represents the best approach at understanding these events.

A leading hypothesis is that mineral phase transformation at high pressure and temperature densifies the material, leading to local normal stress drops and damage zones that can nucleate dynamic fractures [1,2]. Heat generation from the fracture may increase the rate of phase transformation, aiding in a runaway reaction that can generate an earthquake.

We model a subducting plate in central Japan using a thermo-mechanical extended finite element method. The finite element model includes slab plasticity as well as a phase transformation based on the stress and temperature. This leads to a densification of the “undeformed” state as well as heat production. Fracture is initiated at bounding surface, which in later version of the model will be stress and temperature dependent. Initially, we try to fit the model to small-scale experiments conducted at GSECARS beamlines at the Advanced Photon Source. We then apply the model to see whether tremors resembling earthquake records can be generated.

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Multiscale Modelling of Normal Fault Rupture-Soil-Foundation Interaction

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Key Words: *Multiscale modelling, finite element method, discrete element method, normal fault rupture, soil-foundation interaction*

A multiscale approach [1] that couples the finite-element method (FEM) and the discrete-element method (DEM) is employed to model and analyse the earthquake fault rupture-soil-foundation interaction (FR-SFI) problem. In the approach, the soil constitutive responses are obtained from DEM solutions of representative volume elements (RVEs) embedded at the FEM integration points so as to effectively bypass the phenomenological hypotheses in conventional FEM simulations. The fault rupture surfaces and shear localization patterns under normal faults with or without foundation atop have been well captured by the multiscale approach and verified with available centrifuge experimental [2] and numerical results [3]. By examining the responses and microstructural evolutions of local RVE packings, it is found that the RVEs located in- or outside the shear bands behave distinctly, and may change their stress states from initial at-rest to active in the normal fault case. The micromechanics study also sheds lights on the capability of heavy foundations in protecting the superstructure as a result of rupture surface diversion.

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Numerical study on the hydrate rich sediment behaviour during depressurization

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Key Words: Gas pressure, depressurization, multi-phase flow, saturation, THMC

Natural gas hydrates have been investigated for past several years as a potential resource for commercially producing gas. The stable condition for the formation of gas hydrates sediments i.e., high pressure and low temperature generally occurs in deep-sea and permafrost regions. The methane gas extraction from the hydrate-bearing sediments was carried out by drilling and using various dissociation methods. The dissociation methods include thermal injection, depressurization, and chemical injection, which will cause a significant loss of solids in the pore space of geomaterials after extraction. The loss of solids will eventually reduce the reservoir strength, leading to borewell wall collapse, causing subsurface landslides (Collett et al., 2002).

The behavior of gas hydrate sediments is governed by coupled Thermo-Hydro-Chemo-Mechanical (THMC) response during the gas extraction process. In this study, in order to understand the coupled behavioral response of hydrate rich sediments, a 2D hydrate reservoir is simulated (using a multi-phase numerical schema) and analysed under axis symmetric conditions. The initial results suggests that the rate of change of gas pressure near the well bore decreases with the increase in the duration of the extraction. Further, the maximum settlement occurs near the seabed level while the rate of settlement decreases with time. The maximum shear stress generally occurs near the well bore which results in associated maximum volumetric strains. Thus, the continuous gas extraction results in highly porous medium which is stabilized primarily due to the geomechanical changes.

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On the frictional dissipation of micromechanics-enhanced phase-field model

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Key Words: *Phase-field Method, Rock Friction, Micromechanics, Nonlinear Yield Criterion*

A micromechanics-enhanced phase-field model (MicroPFM) proposed by You et al. (2021) recently is capable of better describing lower scale (mesoscale) features of fracture in quasi-brittle rocks, for instance microcrack growth and frictional sliding along the lips of microcracks. However, on the one hand, the frictional dissipation in this homogenization-based model vanishes, and this counterintuitive behavior was accused of using associative flow rule in the evolution of inelastic strain (Ulloa et al, 2022). On the other hand, the involved linear yield function in the MicroPFM underestimates rock strength under no or low confining pressure. Driven by these problems, we first present a new dissipation mechanism during frictional sliding of microcracks at the mesoscale, and then build a macroscopic phase-field model grounded in various microstructure mechanisms by using the energy equivalence principle. Several validation cases spanning two different scales confirm that the frictional dissipation can be retrieved by an appropriate Helmholtz free energy function, where even an associative flow rule is employed. Furthermore, by specifying the frictional dissipation coefficient, a suit of nonlinear yield criterion is proposed to uniformly capture the crack initiation, peak strength and fault slip envelops of rock. Three examples corresponding to Beishan granite, Lac du Bonnect granite and Carrara marble respectively are investigated to show desirable predictive capability of the proposed nonlinear yield criterion, in particular, when the tension cut-off behavior is involved.

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Phase-field Modeling of Nucleation and Propagation of Geologic Faults

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Key Words: Phase-field method, Fault rupture, Shear fracture, Fracture mechanics, Frictional contact

Earthquakes are among the deadliest and costliest natural hazards. Earthquakes are associated with unstable slip on surfaces of discontinuities within the Earth's crust, known as faults. The faulting process involves not only rate- and state-dependent frictional sliding along a fault but also complex evolution of discontinuous geometry such as kinking, branching, and intersecting of faults. Further, fault rupture often gives rise to off-fault damage, which cannot be readily captured by discrete approaches to fault geometry and need to be defined separately through a supplementary bulk constitutive relation. For these reasons, numerical simulation of fault rupture dynamics has long been a notoriously challenging problem in computational mechanics and geophysics alike. Here, we present a phase-field approach to computational modeling of fault nucleation, growth, and propagation, which is built on recent phase-field formulations for quasi-static shear fractures with frictional contact [1, 2]. Compared with existing approaches for the same purpose, the phase-field approach has two main advantages: (i) it can handle complex geometry of faults without any topology-tracking algorithms, and (ii) it can capture both fault propagation and off-fault damage in a unified way. We have verified the new phase-field method using the problem of an anti-plane dynamic rupture on a strike–slip fault, comparing its results with those from a discontinuous approach, namely, the finite element-spectral boundary integral scheme [3]. We then demonstrate the capabilities of the phase-field method for modeling fault propagation problems that involve complex features from kinking and intersecting to off-fault damage.

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Prediction of Rate-dependent Mechanical Behaviour of Toyoura Sand Employing a Newly Proposed Visco-plastic Constitutive Model

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Key Words: S*train rate effect, Visco-plastic model, Rate-dependent response, Drained, Triaxial test, Sand*

Response of soil under medium to high strain rate loading has been of consideration for several military and civilian applications such as air blasts and explosions, projectile penetration, dynamic compaction, pile driving and rapid load testing of piles etc. The mechanical behaviour of sand has been noticed to differ significantly in transient tests with strain rate ranging between 10^{-5}/s to 1/s or even higher [1]. Such rate effects may further vary with density state of the sand and applied level of confinement. Rate effect in sand is generally manifested by an apparent enhancement of soil strength and stiffness primarily due to suppressed particle re-arrangement, increased viscous and inertial effects associated with the higher ranges of strain rate. For modelling and design of geotechnical applications involving medium to high strain rate loading, it becomes imperative to consider the rate-dependent constitutive response of the soil. The rate-dependent material models are often formulated within a general framework of elasto-viscoplasticity involving Perzyna [2] type overstress concept. In this regard, recently Mukherjee et al. [3] proposed a 3D non-associative overstress model, which incorporates both shear and volumetric strain based hardening/softening response and aptly captures some of the key features observed during experiments on sand involving higher strain rates. Such behavior includes strength enhancement with distinct peak followed by rate induced softening and reduced compression; however, the predictability of the proposed model was examined for a limited triaxial test data on coral and silica sand, and primarily focused on strain localization phenomena under biaxial loading condition.

In the present study, the visco-plastic model proposed by Mukherjee et al. [3] has been further assessed over different ranges of confining pressure and strain rate in reference to the drained triaxial experimental results available for Toyoura sand [1, 4]. The influence of strain rate on peak strength, friction angle and strain at peak strength has been analyzed in detail based on the model predictions at three different density states. An increase in peak shear strength of around 60% has been observed for dense Toyoura sand over four orders of magnitude increase in the logarithmic scale of strain rate; whereas, such increase has been limited to 40% and 20% in case of medium dense and loose state, respectively. The corresponding increase in the peak friction angle has been found to be around 20-15% for a change in density state from dense to loose one. However, the rate-induced enhancements noted in both the peak shear strength and friction angle has been observed to remain nearly independent of the level of confinement, except for loose state where such enhancement is more pronounced at lower confinements. For dense state, the strain at peak strength increases with increasing strain rate indicating a delayed peak; whereas, an early peak has been observed for medium dense to loose Toyoura sand at higher rates implying decrease in the magnitude of strain at peak strength.

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Stochastic Homogenization of Large Deformation Plasticity in Porous Brittle Solids

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Key Words: Material Point Method, Microstructure-Based Modeling, Gaussian Random Field, Finite Strain Elastoplasticity, Porous Brittle Solids

Porous brittle solids such as rocks, snow and foams exhibit complex mechanical behavior whose origin can be linked to deformation mechanisms on the microstructural level. Understanding the intricate mechanics of such materials is crucial to the modeling of, e.g., avalanche release processes and earthquakes. Upscaling of elasticity and yielding of arbitrary microstructures using the Finite Element Method (FEM) has become a standard procedure. However, numerical methods to study the transition from small to large deformation situations involving irreversible deformations are still rare. Treating such large deformations is feasible for materials with particulate microstructures using the Discrete Element Method (DEM), but most porous media cannot be approximated by such granular geometries. The lack of flexible computational techniques for these materials prevents the development of accurate homogenized constitutive models.

In this work, we use the Material Point Method (MPM) to investigate large deformation mechanics of porous brittle solids characterized by irregular and bicontinuous microstructures where a segmentation into grains and bonds would be ambiguous. Such microstructures are obtained artificially by level-cutting Gaussian Random Fields (GRF), allowing specific structural properties such as the solid volume fraction to be defined beforehand. This GRF-based scheme facilitates a computationally efficient generation of an ensemble of geometrically different microstructures for each set of prescribed structural properties. Finite size effects are minimized by averaging over different realizations for given structural properties. We demonstrate the usability of our stochastic-numerical approach by examining microstructures with a wide range of porosities under compression. We study the full deformation including the microstructural collapse and packing, going beyond yielding and failure onset. Considering ensembles of microstructures, the uncertainty in the stress-strain response is quantified and related to the error in the numerical discretization.

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A Depth-Averaged Material Point Method for the Simulation of Snow Slab Avalanche Release

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Key Words: Snow Slab, Avalanche Release, Material Point Method, Depth-Averaged Model, Elastoplasticity, Critical State Theory

Snow slab avalanches release due to crack propagation within a weak snow layer buried below a cohesive snow slab. In 1979, McClung [1] described this process assuming an interfacial and quasi-brittle shear failure for the weak layer. This model fails to explain observations of propagation on low angle terrain and remote avalanche triggering. To address this shortcoming, Heierli et al. [2] adapted in 2008 the anticrack concept developed for porous rocks to weak snow layers. In 2018, Gaume et al. [3] showed that mixed mode shear-compression failure and subsequent volumetric collapse (anticrack) of the weak layer were necessary ingredients to accurately model propagation mechanisms, thus reconciling apparently conflicting theories. More recently, large scale simulations based on the Material Point Method (MPM) and field observations revealed a transition from slow anticrack to fast supershear crack propagation [4]. This transition, which occurs after a few meters suggests that a pure shear model should be sufficient to estimate the release sizes of large avalanche release zones.

Motivated by this new understanding, we developed a depth-averaged MPM for the simulation of snow slab avalanches release. Here, the weak layer is treated as an external shear force acting at the base of the slab and is modeled as an elastic quasi-brittle material with residual friction. We first validate the model based on simulations of the so-called Propagation Saw Test (PST) and comparing numerical results to analytical solutions and 3D simulations. Second, we perform large scale simulations and analyse the shape and size of avalanche release zones. Finally we apply the model to a complex real topography. Due to the low computational cost compared to 3D MPM, we expect our work to have important operational applications for the evaluation of avalanche release sizes required as input in hazard mapping model chains. Finally, the model can be easily adapted to simulate both the initiation and dynamics of shallow landslides.

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Computational mechanics for snow and avalanche modeling

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Key Words: *Snow, Avalanches, Computational Mechanics, MPM, DEM*

Snow is a complex material which can sustain stresses like a solid or flow like a fluid depending upon the load it is subjected to. Snow avalanches result from a complex stick to slip failure mechanism in a layered snowpack. Once in motion on a mountain slope the collective behavior of snow particles lead to complex and transient flow dynamics. Quantitative and accurate prediction of slope failure, avalanche release sizes, run-out distances and impact pressures can be based on numerical solution of partial differential equations as well as appropriate constitutive models. Over the last 2 decades, the increase in computational capabilities and the development of advanced numerical models enabled the relaxation of several simplifying assumptions. These models contributed to a significant improvement of our understanding of snow and avalanche mechanics. Here, selected and recent numerical methods for computational snow and avalanche mechanics at high strain rates are presented. Particular emphasis is placed on the Discrete Element Method and the Material Point Method for application at different scales. At the scale of snow microstructure, combining X-ray computer tomography or stochastic microstructure reconstruction techniques with numerical mechanical models has allowed to gain crucial insights into the mechanics of snow under various loading modes. Through homogenization techniques, these numerical results helped to develop constitutive snow models. At the mesoscale, numerical models for large deformations allowed to reproduce (anti)crack propagation mechanisms involved in snow slab avalanche release. At the slope scale, recent models were able to simulate both avalanche release and flow in three dimensions in a unified manner. Additional applications and developements include avalanche impact pressures, wave phenomena, snow-vehicle interaction, avalanches in forested terrain and depth-averaged modeling. Suggestions for future research include more complex rate-dependent constitutive models for dry and wet snow, modeling wet slab and glide-snow avalanches which could become more frequent due to global warming, the effect of spatial variability of snow mechanical properties, as well as model inter-comparisons.

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DEM investigation of crack propagation regimes in large-scale snow fracture experiments

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Key Words: *Discrete element method, Dry-slab avalanche, supershear crack propagation.*

Avalanche accidents mainly occur due to dry-snow slab avalanches. Their release is a multi-scale process which starts with the formation of a localized failure in a highly porous weak snow layer underlying a cohesive snow slab, followed by rapid crack propagation within the weak layer. Finally, a tensile fracture through the slab leads to its detachment. The dynamic process of crack propagation which affects the size of avalanche release zones, is still rather poorly understood. Here, we use a 3D discrete element method (DEM) to numerically simulate fracture mechanical tests commonly called Propagation Saw Tests (PSTs) and analyze fracture dynamics using a micro-mechanical approach. Using cohesive and non-cohesive ballistic deposition, we numerically generate a highly porous, brittle weak layer underneath a dense cohesive slab. First, our DEM model is used to reproduce precisely the PST behavior extracted from experiments based on Digital Image Correlation. Our results show that a stationary crack propagation speed regime appears if the snow column is long enough. Elastic moduli of the slab and weak layer as well as weak layer shear strength are key variables influencing crack propagation by affecting the critical crack length for the onset of crack propagation, and the crack velocity. Our results highlight the effect of these mechanical parameters on the propagation distance required to obtain a steady-state regime and their implication on dry-snow slab avalanche release. In addition, our numerical experiments show the apparition of a so-called supershear crack propagation regime for steep slopes in which the crack velocity becomes intersonic. Overall, our results lay the foundation of a comprehensive study on the influence of snowpack mechanical properties on the fundamental processes of slab avalanche release.

Modelling Roll Waves and Erosion-Deposition Waves in Snow Avalanches with the Material Point Method

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Key Words: *Roll Waves, Erosion-Deposition Waves, Snow Avalanches, MPM*

Roll waves can lead to severe flow variations and deep flow depth, which have been one of the key concerns in many artificial and natural flows composed of water and/or granular materials [1]. Recently, surges called erosion-deposition waves have been identified from dry granular flows [2]. Compared to roll waves which have moving material between the wave crests, erosion-deposition waves have completely stationary regions between individual crests. Although frequently observed from experiments and field events, roll waves, erosion-deposition waves and their transitions are challenging to be modelled under real-scale conditions involving complicated terrain and flow dynamics. In this study, we simulate the roll waves and erosion-deposition waves in snow avalanches by using the material point method (MPM) and an elastoplastic constitutive model based on critical state soil mechanics. In particular, a snow avalanche at Vallée de la Sionne (VdlS) in Switzerland is modelled with consideration of bed erosion. The properties of the simulated snow are firstly calibrated with the deposition depth of the VdlS avalanches measured with a laser scanner. The dynamic behaviour of the avalanche is then analysed in terms of the different waves, the flow depth evolution at a fixed location, as well as the temporal and spatial evolution of the flow velocity. It is observed that both roll waves and erosion-deposition waves are naturally captured from the simulated avalanche. The flow depth evolution from the simulation shows satisfactory agreement with the field data measured with FMCW radar. The model is also able to recover the spatial evolution of the wave activity from release to deposit, which was measured in the field experiment using a radar. With both the numerical and field investigations, this study offers new perspectives on wave behaviour and provides a validated numerical approach for exploring waves in granular flows like snow avalanches.

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MPM×DEM method to model multiscale cohesive granular process involved in snow avalanches.

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Key Words: Multiscale MPM×DEM, granular flow, free-surface, avalanches

Snowpack can be characterized as a loose granular assembly of cohesive non-spherical particles, whose shape and size can greatly vary depending on meteorogical conditions and depth of the considered snow layer. Recent discrete elements (DEM) simulations of centimetric snow samples [1] have highlighted a complex mechanical response, including strong strain-softening and volumetric collapse. Moreover, these features are sensitive to the wide variety of microstructural patterns observed in snow. Avalanches, on the scale of a mountainslope, involve large deformations and can propagate over hundreds or thousands of meters. For modelling such large scale processes, while preserving proper account of microstructural effects on snow mechanical response, a double-scale MPM×DEM approach is proposed (where MPM stands for Material Point Method). Hence, MPM performs the resolution of large scale free-surface flows by relying on a rheology obtained from a homogenized numerical constitutive law (HNCL). Each Gauss point embeds its own "realistic" microstucture handled by a DEM approach. The HNCL is expected to capture the complex mechanical behavior of the material in a more robust and realistic manner than any macroscopic analytical constitutive model. Our coupling strategy differs from another recent MPM×DEM implementation [2], in particular with respect to the periodic boundary conditions [3] used at the DEM scale. Benchmark simulation results (slump tests) will be presented to evaluate the approach. Then, typical slab-weak layers systems involved in slab avalanche release will be modeled. The influence of initial snow microstructure will be investigated using 3D microtomographic images of different snow samples as inputs for the DEM samples.

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New insights on avalanche release mechanics based on large-scale elastoplastic simulations

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Key Words: Snow Slab Avalanche Release, MPM, Elastoplasticity, Critical State Theory, Anticrack, Supershear, Crack Propagation

The release of snow slab avalanches starts with the failure of highly porous weak layer buried beneath a cohesive slab leading to mixed-mode crack propagation along the slope. The first modelling attempt of the process date back to 1979 with a pure shear weak layer fracture assumption proposed by McClung [1]. Later, Heierli [2] extended the concept of anticrack, to account for weak layer volumetric collapse and subsequent slab bending. Recent advances [3] reconciled these approaches and have shown the existence of a supershear crack propagation regime leading to intersonic propagation speeds [4].

Here, based on the Material Point Method, finite strain elastoplasticy and critical state theory, we report a transition from sub-Rayleigh anticrack to supershear crack propagation involving the Burridge–Andrews mechanism. The existence of this transition is further confirmed by full-scale avalanche analyses. By accounting for slab fracture, we highlight that soft slabs can prevent supershear transitions to occur. In addition, it is shown that crack branching in the slab can either occur from top to bottom in the case of slow propagating anticracks or from bottom to top for supershear cracks. Through a sensitivity analysis, we investigate the conditions for crack arrest or so-called 'en echelon' slab fracture. Full 3D simulations reveal interesting propagation and release patterns related to the interplay between cross-slope and down/up-slope propagation and slab tensile failure. This enables to analyse slab fracture modes at crown, flanks and staunchwall of the avalanche. These findings allow us to reach a next step in our understanding of the release mechanics in order to predict avalanche release shapes and sizes.

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New Perspectives for the Elasto-Plastic Modelling of Snow

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Key Words: Snow Mechanics, Constitutive Model, Elasto-Plasticity

Modelling the mechanical behaviour of snow for laboratory or in situ conditions requires advanced constitutive relationships that are able to account for large inelastic deformations, viscosity, rate dependency, material and geometrical non-linearities, etc. All these aspects characterize the response of a snow element with respect to external actions and strictly depend on the peculiar properties of snow at the micromechanical scale, such as: the presence of bonds between grains (sintering), the effect of the temperature gradient on the grain shape (metamorphisms), etc.

Therefore, the elasto-plasticity theory was largely adopted for snow mechanics purposes, often starting from models originally conceived for soils (e.g., the modified Cam-clay) [1, 2]. The existing models have often a limited range of application only for some specific types of snow (e.g., rounded grains or faceted crystals) while new ones need to be more general. For instance, in the new elasto-plastic models for snow, the yield locus is required to be highly deformable and also capable of varying its shape to follow different stress paths both in the deviatoric and in the meridian plane.

In this work we analyse the possibility of adopting a tailored version of the Bigoni-Piccolroaz yield function for snow [3]. Moreover, we introduce three hardening/softening laws for snow that consider the effect of: i) irreversible volumetric deformations, ii) bonding/degradation processes, and iii) rate dependence. Finally, we depict some concepts related to the numerical implementation of these topics in the framework of a continuum model for snow developed for Finite Element (FE) analyses.

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The effects of precipitation particle shape on snowpack

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Key Words: *Precipitation particle shape, Snowpack, Discrete element Method*

Snowflakes reflect meteorological information in the sky such as the temperature and degree of supersaturation, and their shape is formed by the balance of them. These shapes affect not only how the snow falls (*e.g.* snow-fall speed [1]), but also how the snowpack is formed. Although these shape differences of precipitation-particle are negligible after mechanical- and thermal-induced metamorphosis in snowpack, it causes differences in the mechanical property of snowpack in the early stage of them. In addition, it is said that some kinds of precipitation-particle from cyclone form weak layer within the snowpack, which causes a potential occurrences of surface avalanches over broad area simultaneously [2].
Our interest is to understand the snowpack properties caused by the differences of precipitation-particle and environmental conditions from the granular scale. For examples, the effects on snowpack with/without rimed snow crystal and with/without wind. In nature, it is difficult to observe the desired precipitation-particles freely in controlled environmental setting. In order to solve these problems, numerical granular sedimentation experiments with non-spherical grains are conducted. Clump particles constructed by spheres are employed to resemble precipitation-particles in discrete element method (DEM) [3]. To make granular packing, free fall of clumps are simulated with changing the shape of clumps and initial conditions (initial orientation and initial velocity/rotational velocity) as parameters.

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Predicting contact force chains within granular materials using machine learning methods

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Key Words: *Granular materials; Contact force chains; Machine learning; Artificial neural network*

There is a dearth of machine-learning investigations of the micro-mechanics of granular soils. The micro-mechanics deals with the mechanics of granular materials at the micro-scale (often particle scale) or meso-scale and is contrasted with the macro-mechanics which focuses on the macro-scale behavior measured at the laboratory sample scale or field scale. In this paper, a novel investigation of the contact force chains (CFC) in quasi-statically sheared granular materials using machine learning methods is conducted. An artificial neural network (ANN) based on discrete element method (DEM) simulation data is developed and applied to predict the anisotropy of CFC in an assembly of spherical grains undergoing a biaxial test. Five particle-scale features including particle size, coordination number, x- and y-velocity (i.e., x and y-components of the particle velocity), and spin which all contain predictive information of the CFC are used to establish the ANN. The results of model prediction show that the combined features of particle size and coordination number have a dominating influence on the CFC estimation. An excellent model performance manifested in a close match between the rose diagrams of CFC from the ANN predictions and DEM simulations is obtained. In addtion, some preliminary results of the prediction of the constitutive response of granular materials using the machine learning method are also presented. Our ongoing work includes the direct prediction of the inter-particle contact forces of a real granular material (such as sand) based on the micro computed tomography input, and the machine learning based constitutive modelling of granular materials.

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Predicting Pile Bearing Capacity with Machine Learning

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Key Words: Standard Penetration Test, Pile Capacity, Machine Learning

For the past years, machine learning (ML) techniques have been applied to several engineering areas, including geotechnics. Although there are studies dedicated to pile capacity prediction, many gaps still remain in this research field, like the use of few ML techniques, datasets with few examples and poor variety of soils. To fill some of these gaps, this work presents an application of ML techniques for predicting the bearing capacity of precast concrete pile foundations.

The raw dataset, collected from the literature, contains 165 load test results and its respective SPT sounding data. Four datasets based on different semi-empirical methods and one aggregating all inputs were created and used to train seven different ML algorithms. The leave-one-out cross validation approach was used for training and testing, for its ability to better explore the information within the dataset. We use the root-mean-square deviation (RMSE) and the coefficient of determination (R^2) as metrics to evaluate the ML techniques. The table below summarizes the best results obtained from the study, comparing some of the tested ML techniques with classical semi-empirical methods from the literature.

Random forest (RF) presented best performance for both R^2 and RMSE, followed by k-nearest neighbor (KNN). The best semi-empirical method was [1] with respect to R^2, the only one that overcame linear regression (LR). [2] and [3] presented the worst performance. One can also notice that the semi-empirical methods presented high RMSE comparing to all other techniques. It is worth commenting that RF was the best technique not only in the presented table, but in most tests varying input combinations and datasets. After testing alternatives for KNN, we concluded that the best approach is simply weighting point distance.

Method	R^2	RMSE
RF	0.770	635.96
KNN	0.762	651.24
[1]	0.756	1443.11
LR	0.728	708.25
[2]	0.660	896.10
[3]	0.614	922.34

From these results, one can conclude that ML techniques are capable of modeling this type of problem. We suggest for future works the investigation of different input combinations, using information like the cone penetration test (CPT), and including other types of piles.

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Application of Strain Space Multiple Mechanism Model Accounting for Inherent Anisotropy to Seismic Response of Soil-Structure Systems

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Key Words: *Strain Space Multiple Mechanism Model, Soil-Structure System, Seismic Response, Inherent Anisotropy*

Consideration of inherent anisotropy is crucial to gaining an improved understanding of the behavior of granular materials. Inherent anisotropy is thought to arise from the preferred particle arrangement and contact orientation of granular materials during sedimentation. Although inherent anisotropy of granular materials has been a subject of extensive investigation for almost 40 years, only a limited number of studies have investigated the effect on the dynamic behavior of soil-structure systems during earthquakes [1].

This study aims to investigate the inherent anisotropy's effect numerically on the seismic response of soil-structure systems using the strain space multiple mechanism model that has been extended to account for inherent anisotropy [2]. In the proposed model, three parameters have been introduced to control the degree of inherent anisotropy and its principal direction. Considering the design case studies of port structures [3], the following soil-structure systems are picked up for consideration: breakwater, sheet-pile quay wall, and gravity type quay wall.

The seismic response analyses for the sheet-pile and gravity type quay walls demonstrate that the consideration of inherent anisotropy affects not only the horizontal displacement of the structure but also the excess pore water pressure in the liquefiable deposits. In the case of the breakwater, the vertical strain of the liquefiable layer below the breakwater is affected by inherent anisotropy, resulting in a different amount of breakwater settlement. The above analysis results indicate that the effect of inherent anisotropy cannot be ignored in evaluating the dynamic behavior of soil-structure systems during earthquakes.

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Effective Stress Analysis Method for Unsaturated to Saturated Porous Media and its application to Underground Structure in Liquefiable Ground

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Key Words: *Partially Saturated, Liquefaction, Effective Stress Analysis, Underground Structure*

Background

In recent years, a large number of the unsaturated soil structures such as embankments and slopes were severely damaged due to the multi geotechnical hazards induced by rainfall and earthquake (2004 Niigata-ken Chuetsu Earthquake, 2018 Hokkaido Eastern Iburi Earthquake, etc). Numerical analysis considering the characteristics of unsaturated soil is a promising approach to analyse the effects of combined disasters. Hence, an effective stress analysis method for analysis of both unsaturated and saturated porous media and the transition from unsaturated to saturated soil is developed. This study shows validation of the developed analysis method and its application.

Modelling for unsaturated soil

To consider the characteristics of unsaturated soil, simplified three-phase effective stress analysis was conducted. This method uses the equivalent bulk modulus of fluid considering the degree of saturation and the specific moisture capacity assuming that the pore air pressure equal to atmospheric pressure [1][2]. The suction is defined as the negative value of the pore water pressure, and it is related to the increase in the initial value of the yield surface.

Validation analysis and application to multi geotechnical hazard

To validate the developed analysis method, 1D leaking test and the quasi 1D non-steady seepage flow through soil was idealized. The numerical results reproduce the spatial and temporal distribution of pore water pressure.

Furthermore, the seismic behaviour of an underground structure surrounded by unsaturated and saturated liquefiable ground with three different ground water level, were estimated as examples for comparison. Non-linear response of the reinforced concrete, the relationship between stress and strain for concrete and rebars, is considered as well.

The pore water pressure in unsaturated layer increases, and a part of the unsaturated layer near the ground water level changed into saturated soil. The deformation of the underground structure is larger at the boundary of the unsaturated and saturated layers.

Conclusion

The following conclusions are obtained: (1) the proposed method of incorporating the characteristics of unsaturated soil is verified, (2) the simulation well represented the seismic behaviour of the excess pore water pressure and the deformation of the RC structure in unsaturated layer on liquefaction.

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Evaluation of Wave-Resistant Stability of Suction Bucket Foundations with Different Foundation Dimensions

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Key Words: *Suction Bucket Foundation, Effective Stress Analysis, Monotonic and Cyclic Loading, Wind and Wave Resistant Stability*

Suction bucket foundations have been attracting attention in recent years as a foundation method for offshore wind power facilities. To investigate the foundation stability against wave loading, Nielsen et al. carried out monotonic and cyclic loading tests using a small-scale mono bucket foundation installed in water-saturated dense sand [1]. Ueda et al. performed two-dimensional effective stress analyses to examine the foundation's wave-resistant stability; the seismic behavior was also investigated through shaking table tests in a centrifugal field [2]. However, the effect of different bucket dimensions (e.g., bucket diameter) on wave-resistant stability has not been thoroughly investigated.

The present study aims to numerically investigate the bucket dimension effect on the foundation's wave-resistant stability using two-dimensional effective stress analyses under undrained and partially drained conditions. A number of combinations of different monotonic and cyclic horizontal loads are applied for two types of suction bucket foundations with different bucket diameters installed in a liquefiable sandy deposit. Whereas the buckets are modeled as linear beam elements, the strain space multiple mechanism model [3] is used to consider the nonlinear response of the ground with pore water pressure increase during the cyclic loading.

Referring to Nielsen et al. [1], the computed inclination angle of the foundation after the combined loading is organized as a contour map on the drawing where the horizontal axis is the amplitude of monotonic loading while the vertical axis is the amplitude of cyclic loading. It is noted that both axes are normalized by the ultimate load obtained from pushover analyses (i.e., drained monotonic horizontal loading). The contour maps demonstrate that the bucket diameters affect the inclination angle under wave loading. Preparing such contour maps for foundations with different bucket dimensions makes it possible to easily and visually evaluate the degree of foundation inclination under any combination of monotonic and cyclic loads.

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High-performance solid-fluid coupled dynamic simulation of soil liquefaction

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Key Words: *high-performance simulation, solid-fluid analysis, soil liquefaction, Cycliq constitutive model*

This study develops an efficient solid-fluid coupled simulation method of soil liquefaction analysis, based on the GEOSX open-source, multiphysics simulator. Solid-fluid analysis is achieved through an explicit FEM-FVM coupling routine. The CycLiq constitutive model is implemented for the simulation of soil liquefaction behavior, based on the cutting plane stress integration algorithm and the three-dimensional mapping rule. LEAP-UCD-2017 centrifuge shaking table tests are simulated to validate the soil liquefaction analysis method. Moreover, an underground tunnel model with large-scale gravel piles is simulated to demonstrate the simulation ability of 10 million degrees of freedom solid-fluid coupled dynamic liquefaction analysis. The efficiency and scalability of the high-performance solid-fluid coupled analysis method is evaluated by varying the scale of the analysis model. The results highlight that proposed method can significantly expand soil liquefaction analysis capability in terms of both problem size and solution fidelity.

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Importance of Appropriate Liquefaction Resistance Simulation for Underground Structure Seismic Response Analysis

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Key Words: *Liquefaction resistance, Underground Structure, Seismic Response Analysis*

This study investigates the importance of appropriate liquefaction resistance simulation for underground structure seismic response analysis in liquefiable ground. A series of numerical simulations are conducted using solid-fluid FEM with two constitutive models for soil liquefaction analysis. The first constitutive model is the original CycLiq model proposed by Wang et al. (2014) which is able to provide good simulation for the post-liquefaction behavior of sand, but tends to underestimate liquefaction resistance at low cyclic stress ratio. The second model is proposed based on the original CycLiq model to enhance the description of the liquefaction resistance. These two models are first used in the simulation of the centrifuge shaking table test conducted by Zhu (2021) for validation. Upon validation, the models are used in the simulations with different input peak acceleration amplitudes (PGA) to evaluate the influence of the models' ability to appropriately reflect liquefaction resistance on the seismic response analysis of underground structures. The analysis results show that these two models can produce similar response of underground structure in liquefiable ground within a certain range of PGA. However, the original model overestimates the response of underground structure at low PGA and underestimates it at high PGA, compared with the modified model. The results suggest that it is important for constitutive models to accurately reflect the liquefaction resistance of sand when simulating the seismic response of underground structures. The influence of liquefaction resistance on the seismic response of above ground structure needs to be further studied.

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Seismic behaviour of embankment containing multi-segmented rigid bodies placed on liquefiable ground

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Key Words: *Multi-segmented rigid bodies, Liquefaction, 3D effect of dynamic SSI*

Three-dimensional effect of dynamic soil-structure interaction (SSI) on liquefiable ground critically matters in the embankment containing the underpass structure. Damage closely related to this effect has been reported in Mid Niigata Prefecture Earthquake in 2004 [1] and the 2016 Kumamoto Earthquake [2]. In these earthquakes, the joint openings of the box culverts occurred due to the liquefaction of the foundation ground; the damage patterns have been unstructured.

A three-dimensional model of a road embankment containing a box culvert with joint was fabricated on liquefiable ground. Its seismic behaviour was investigated with geotechnical centrifuge of 50G. To visualize the foundation ground under the culvert, a half-section embankment-culvert model was used. The longitudinal section was observable from the front.

The testing result reproduced the past-reported joint opening: joint opened as if it was inclining toward the culvert-mouth as liquefaction progressed. The 4 locations of the excess pore water ratios directly under the culvert-mouth, the joint, and the shoulder and the centre of embankment were respectively compared. The measured results indicated that the excess pore water ratios under the culvert exceeded that under the embankment in each point, and its ratio under the joint exceeded under the culvert-mouth; they can be categorized as 3D effect of dynamic SSI.

In summary, liquefaction is more likely to occur in the foundation ground directly under the culvert. This different progress of the liquefaction under the culvert and the embankment seems to amplify the joint opening of the box culvert. In the future, we plan to conduct reproductive analysis to verify whether this interesting response can be confirmed in the numerical analysis.

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Seismic response of sheet-pile structures in liquefiable soils: Stochastic modeling and validation

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Abstract:

Design of sheet-pile walls in granular soils is traditionally based on limit equilibrium analysis approaches that are known to be highly over-conservative. An alternative approach that has gaining much popularity in recent years is to use nonlinear elastoplastic analyses that more accurately account for the initial state of soils and the soil-pile interaction. However, majority of the modeling tools available in engineering practice are limited to simplified constitutive models that are unable to properly simulate the cyclic response of soils. Even when more advanced constitutive models are available, their performance has been evaluated against limited number of element tests that cover a narrow range of densities and initial stresses and target specific stress and strain paths that might not be representative of what the soil experiences in its interaction with structures. To address these shortcomings, there is a need for systematic evaluation of constitutive models and numerical modeling techniques against high quality experimental data that cover a wide range of initial stresses, soil densities, and stress/strain paths. Here, seismic response of a sheet pile wall embedded in a liquefiable soil is used to demonstrate the versatility of such a systematic approach. The sheet-pile wall was first designed by conducting a series of nonlinear finite element analyses that considered the coupled response of the pore fluid and soil skeleton and included a critical state elastoplastic model of soil skeleton that was thoroughly calibrated against element test data performed on the selected soil. Seismic performance of the designed sheet-pile wall was then predicted for a large number of target seismic motions. Following these blind predictions, a scaled model of the system was tested in a geotechnical centrifuge. The measured response of the wall was found to be remarkably close to the blind prediction. The computational model, initially validated against the element tests and the centrifuge experiment, was then used in a series of stochastic finite element analyses to assess the response of the system for a wide range of seismic motions and soil densities. The analysis results were compared to extensive experimental results obtained in the course of an ongoing international collaborative research project, Liquefaction Experiments and Analysis Projects (LEAP)[1]. The capabilities and limitations the computational model in capturing the response of the sheet-pile wall structure over a wide range of densities and base motion intensities and frequency contents are discussed.

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A coupled BCHM model for MICP treatment in soil

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Key Words: MICP, BCHM Coupling, Multifield Problem, FEM

Microbially induced calcite precipitation (MICP) provides potential of developing sustainable methods for improving the engineering properties of soil. MICP treatment in soil can cause complex interactions among different fields, by which ureolytic bacteria are utilized to catalyze urea hydrolysis, producing ammonium and carbonate ions. With the presence of calcium, calcite can be precipitated. In soil, the filling of calcite in the pore spaces can reduce the porosity as well as permeability. Besides, calcite act as binding material among the solid grains which can improve the mechanical stiffness and strength.

In the present study, a coupled bio-chemo-hydro-mechanical (BCHM) model is developed with the aim on a better understanding of coupling effects involved in MICP. In this model soil is considered as saturated porous media. The computational domain is a representative elementary volume (REV), in which the solid phase and the liquid phase are considered. In the liquid phase, multi-component transport is considered and described by reactive mass transport equations. The governing equation for the flow process is derived based on the mass conservation of the liquid phase. The couplings between the mechanical and hydraulic fields are incorporated in the mass balance equations for solid and liquid phases. The decrease of permeability following the MICP induced porosity reduction is considered using a modified Kozeny-Carman equation. Modified Cam-Clay model with combined volumetric-deviatoric hardening is adopted to describe the elasto-plastic behaviour of the soil. The increase of stiffness and strength is considered with the calcite-contents-dependent increase of elastic modulus and extension of the yield surface. Besides, the degradation of calcite bonds is considered by introducing a degradation parameter. The model is solved by the finite element method (FEM) based on the open source code OpenGeoSys (OGS). To consider the multifield problem, subsystems for reactive mass transport (BC), flow process (H) and deformation process (M) are defined, respectively. These subsystems are solved iteratively using a staggered scheme [1]. The couplings are considered by defining the dependency of the parameters and variables from different subsystems.

This model has been applied to simulate experiments from different literature sources. The experimentally observed mass and permeability variations in space and time, increase of mechanical stiffness and strength, and the dilatancy behaviour during MICP can be well captured in the model.

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Analysis of coal fluidization mining with continuous-discontinuous element

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Key Words: Fluidized mining, filling rate, filling rate

Comparing to traditional mining methods, in-situ fluidization mining[1] is a promising method for reducing ecological influence. During fluidization mining, coal gangue will be separated from ores and filled back to the excavation region, which greatly reduces strata deformation, depending on the filling rate. Numerical simulations can help the engineers to evaluate the strata deformation and optimize the designs with affordable costs. In this work, a continuous-discontinuous element method[2] is adopted for simulating the coal in-site fluidization mining-filling processes, which is a coupled finite-discrete element methods with explicit integration formulation. The theory of "equivalent mining height" is used to define the backfill mining height. The results partly reveal the influence of filling rate on the strata deformations, surface subsidence and rock burst.

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Analytical quantification of thermal stresses in concrete beams in consequence of multiscale constraints

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Key Words: *thermal stresses, multiscale analysis, eigenstrains, constraints, concrete beams*

Temperature changes in concrete structures result in thermal stresses that may cause cracking. As for concrete beams, these stresses originate from thermal eigenstrains, constrained or prevented at three different scales of observation, namely, the microstructural scale of the concrete material, the cross-sectional scale, and the macrostructural scale of the beams.

The multiscale nature of the thermal stresses is quantitatively addressed by establishing the scale transition (i) from cement paste, sand, and aggregates to the material scale of concrete, (ii) from the material scale of concrete to the cross-sectional scale of the beam considered, and (iii) from the cross-sectional scale to the macrostructural scale of the beam. This mode of analysis is applied to quantifying the fluctuations of microstructural stresses of the concrete constituents for rectangular concrete beams, subjected to thermal loading. Sensitivity analyses, with respect to different heating speeds, different concrete constitutions, different internal relative humidities, and different geometric dimensions of the beams are carried out. This provides better understanding of thermally-induced degradation of concrete structures and helps to improve their durability by optimization of the concrete mixture and improvement of the thermal boundary conditions.

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A coupled implicit MPM-DDA for soil-structure interaction problems

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Key Words: *Material Point Method, Discontinuous Deformation Analysis, Implicit Scheme, Soil-Structure Interaction*

Numerical analysis of the soil-structure interaction problems in a large deformation range is important to understand both the failure mechanisms and the post-failure behaviors of slopes and earth structures. For this purpose, coupled continuum-discrete analysis methods have been developed intensively during the last decade. Those methods mainly employed particle-based methods (e.g., Smoothed Particle Hydrodynamics and Material Point Method) for the modelling of large deformation of soil and discrete element methods (e.g., Distinct Element Method and Discontinuous Deformation Analysis) for the modelling of structures and rigid bodies, where the contacts between them are considered [1, 2].

The previous methods often use an explicit time integration and/or a staggered coupling scheme that alternately runs the continuum method and the discrete method while exchanging the forces and the kinematics. This is owing to the explicit time integration scheme used in the particle methods and/or the Distinct Element Method. However, when we analyze the pre-failure process that is often quasi-static as well as the post-failure behavior, the explicit scheme often exhibits large computational costs due to the limitation of time increment size.

In this study, we newly developed a coupled analysis method of the implicit Material Point Method (MPM) for soil and the Discontinuous Deformation Analysis (DDA), which is an implicit type of discrete element method for structure. The contact between the MPM and the DDA is formulated based on the penalty method, and the equilibrium of the whole system is solved monolithically. Since the Newmark type implicit time integration is used in both MPM and DDA, the fully implicit feature is retained also in the coupled analysis. The developed method was applied to a simulation of a benchmark experiment [3] and the validation was investigated.

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A unified signed-distance-field DEM framework for arbitrary particle shapes

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Key Words: Discrete element method, Irregular-shaped, Signed distance field, Contact potential, Spherical harmonics.

This work develops a signed distance field (SDF)-based contact approach to the discrete element method (DEM) for modeling generic irregular-shaped particles. It is proposed to implement particle models from an SDF-based generic interface that provides an SDF function and a surface projection function. The signed distance is positive inside particles, and vice versa; thus the zeroth isosurface of SDF represents particle surface. With particle surface discretized into a set of nodes, the node-to-surface algorithm is adopted for contact detection, namely, by checking the distance signs of the surface nodes of one particle with respect to another. Then, the energy-conserving contact theory is adopted to derive the contact interaction forces, with the contact potential defined on each intruding nodes. Based on the SDF-based contact framework, particle models are developed based on classical geometries, including poly-super-ellipsoid, poly-super-quadrics, spherical harmonics, and polyhedron; and the existing level set particle model is also integrated. In addition, a weighted spherical centroidal Voronoi tessellation-based scheme is developed for particle surface discretization and reconstruction. Example DEM simulations are provided to verify and demonstrate the capabilities of the proposed SDF-DEM framework. The computational aspects, including the memory consumption and computational efficiency of the approach and aforementioned particle models, are discussed.

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An Improved Extended Material Point Method to Model Shear Band Evolution and Large Deformation Post-failure Behaviors

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Key Words: Extended Material Point Method, Localization detection, Frictional Self-contact, Shear Band, Large Deformation

An improved XMPM formulation is proposed to simulate the evolution of shear bands and post-failure behaviors with large deformations (e.g. landslide). The XMPM introduces a localization search algorithm based on the theory of bifurcation to predict the initiation and propagation of shear band. To deal with the dynamic frictional contact mechanism between the generated shear planes, a formulation of self-contact is integrated into the XMPM framework. In addition, a hybrid implicit-explicit description of discontinuity is considered by employing the level-set method and a point cloud approach to ensure the smoothness of the discontinuity surface during localization propagation. Several numerical examples have been investigated to assess the accuracy and demonstrate the capability of the proposed XMPM approach in simulating the shear band evolution of different engineering problems in both 2D and 3D. The proposed formulation is proven to exhibit minor sensitivity with respect to mesh refinements in predicting the shear-band path. Further research should focus on improving the efficiency and stability of the XMPM solver by considering parallelism and high-order spatial and temporal approximation. It is also interesting to investigate the connection between weak and strong discontinuity in large deformation problems, as well as a variable frictional contact model taking into account the material cohesive and dilatancy characteristics.

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Assessment of Macro and Micro level Heterogeneities for Characterizing Mechanical Behavior of Sand in Biaxial Test employing DEM

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Key Words: *Macro and micro level, Heterogeneity, Biaxial test, Representative volume element (RVE), Wall-based measurement, Sand*

Discrete element method (DEM) is widely used to examine the mechanical behaviour of granular assemblies, like sand, under various loading conditions by performing numerical simulations replicating different laboratory tests. While simulating various element tests from such particle-based methods, it is often required to estimate magnitudes of field variables, such as stresses and strains, which are essentially defined based on a continuum assumption. In this regard, either a wall-based global estimation or a representative volume element (RVE)-based local assessment is often adopted. Wall-based estimation predicts an overall response of the specimen which takes into account only the particle to wall contacts. As a result, such wall-based estimation of field variables is often influenced by the boundary effects arising due to the concentration of stresses and voids around wall boundaries [1], which can be identified as a source for macro level heterogeneities. On the contrary, RVE is considered to be statistically representative of the specimen under consideration. Further, it must be large enough so that an increase in the size will not change the estimated field variables and should exclude any possible macro level heterogeneities. In addition, an RVE should not be too small such that it starts to depict micro level heterogeneities, such as the development of unrealistic localized zones of various field variables due to consideration of only limited number of particles within the RVE [2]. However, deciding the optimal extent of the RVE to avoid such macro or micro level heterogeneities requires a systematic analysis.
In the present study, biaxial test simulations are performed employing DEM with non-circular particles of realistic particle size distribution [3]. Subsequently, an analysis has been carried out to assess the influence of the aforementioned macro and micro level heterogeneities in reference to the characterization of mechanical behavior of the specimen from a chosen RVE configuration. In this regard, a series of simulations have been carried out by generating various RVE configurations with different diameter and volume coverage over the specimen. It has been observed that the wall-based estimation predicts higher stresses and unrealistically higher volumetric strain, particularly at the larger strain levels, in comparison to the RVE-based estimations. However, it is interesting to note that increasing the volume coverage of RVE can predict stresses in the range of wall-based stress estimates. In order to establish a better mechanical characterisation, it has been proposed that the RVE should evolve with the continued deformation maintaining a constant volume fraction coverage in reference to the deformed configuration of the specimen. Further, it is suggested that the RVE should occupy a maximum of 90% volume of the specimen in order to avoid any possible boundary effects and can still be able to capture its overall mechanical behavior. However, when a local variation of field variables is of interest, RVE of smaller diameters can be employed. In such cases, depending on the average particle size of the granular assembly, the diameter of the RVE should be selected ensuring that it is small enough to aptly capture the local variation of field variables and at the same time, large enough to avoid any micro level heterogeneity.

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Detailed Statistical Properties of Cell-Based Packing Structure in Elliptic Particle Systems

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Key Words: Granular Microstructure, Cell-Based Description, Elliptical Particle, DEM

The ubiquity of granular material in nature and in human society makes it important to model, however we are still far from understanding its complex and rich behaviors. One of the difficulties is that the macroscopic granular material properties are sensitive to microscopic structural characteristics. In two dimension, the granular structure can be described in terms of *cell* [1], which is the smallest closed loop in force chains. Recent works revealed the evidence of structural self-organisation and universal statistical properties of cell structure in systems composed of circular particles [2, 3]. On the other hand, particle shape has a great effect on the evolution of granular local structures [4], to which careful attention should be paid.

In this study, we performed numerical simulations, using Discrete Element Method (DEM), to investigate the detailed statistical properties of cell-based packing structure in two dimensional elliptical granular packings. Granular systems of elliptical particles with different particle aspect ratio (quantifies by the ratio of particle long axis to short axis) and intergranular friction, were slowly compressed isotropically into a marginally jammed and mechanically stable state. We found that: (1) The mean coordination number ranges from 3 in very rough particles to 5.5 in very smooth particles which agrees with isostatic theory of non-circular particles. The transition from circular particles to non-circular particles appears when the aspect ratio is less than 1.5. (2) Being different from the result of circular particles system, the initial condition before compression slightly affects the resulting solid fraction in equilibrium even after removing rattlers (floating particles with one or no contact). This may be due to the orientational clustering of elliptical particles [4]. (3) The mean cell volume for each cell order in elliptical particles packs can be interpreted by the extended regular polygon cell model in which the upper and lower bound relations are obtained by the long and short axes of ellipses, respectively.

Our results not only confirm the usefulness of cell-based approach in understanding and modelling the granular materials, but also encourage further using of cell-based approach in non-circular particle systems.

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Discrete Element Simulation on Particle Runout of Dry Granular Chute Flow

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Key Words: *granular avalanches, Discrete Element Method, Power-law*

Avalanches of geomaterials often cause serious damage to downstream area. When the material contains sufficient water, it flows as a fluid, which is called debris flow or mudflows depending on the material type, and its behaviour is investigated as the continuum fluid mechanics framework. On the other hand, when the material is under unsaturated condition, the flow behavior is more like a dry granular flow in which constituent geological grains move individually with mutual interaction [1]. As a result, particles in front of the flow are widely scattered and reach much farther than the mass flow. The evaluation of such '*particle runout*' is important to assure the safety of the downstream area [2].

This study attempts to clarify the particle runout of dry granular chute flow from statistical behaviour of granular materials. We performed a series of 2D Discrete Element simulations for non-circular particles of different particle properties such as particle size, shape, restitution coefficient and friction. We found that (1) the centre of the mass of the deposition tends to be independent from grain shape and size, (2) the distribution of the particle location at the final deposition has a tail of more like a power-law type than an exponential type, and (3) the power-law exponent is affected by the particle size but not affected by the length of the slope. These findings are in accordance with the previous experimental results [3]. The first finding is related to the fundamental rigid block runout model in which the equivalent friction $\mu = H/L$, where H is the height of the slope and L is the horizonal mass runout [4]. As for the finding (2), a simple particle runout model by assuming the Maxwell-Boltzmann type distribution as the initial particle eject speed cannot explain the resulting power-law distribution, and more detailed statistics of individual particle motion should be investigated.

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Evaluation of Skeletal Structure for Binary Granular Mixture Forming Reposed State

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Key Words: *DEM, Angle of repose, Contact force*

Binary granular mixture is composed of two different size particles. The skeletal structure that governs mechanical properties of this material can be divided into three types according to large particle content. These were defined as “Small particle skeletal structure” seen when large particle content is low, “Large particle skeletal structure” found when large particle content is high and “Intermediate skeleton structure” [1]. The authors have been investigating the mechanical properties of binary granular mixtures of large particles with special shapes. In this research, skeletal structure of binary granular mixture composed of large cylindrical particles such as coral gravel and small particles was investigated. First, the angle of repose experiment was reproduced by DEM. Then, three types of skeletal structures were identified from the relationship between the angle of repose and large particle content. This allowed us to evaluate large particle content V_L^b%, which is the boundary between small particle skeletal structure and the intermediate structure, and large particle content V_L^a %, which is the boundary between the intermediate structure and the large particle skeletal structure. Furthermore, the internal structure in the intermediate skeletal structure was analysed from a microscopic point of view.

Based on DEM analysis results, the relationship between the angle of repose and large particle content was analyzed. The boundary large particle content V_L^b% was 15.7%, and V_L^a% was 84.5%. Angle of repose begans to rise from V_L^b, increased to V_L^a, and above V_L^a, the result was same as result of only large particle content (100%). Since this tendency was the same as that of the experiment using the actual material, it was considered that the simulation performed could essentially reproduce the actual experiment. [2].

Here, the contact force equivalent to the own weight of one small particle of $6.99 \times 10^{-3} N$ was used as the reference value, and the relationship between the proportion of contacts below the reference value and the angle of repose was analyzed. With V_L^b% as the boundary, the ratio increased as the angle of repose increased. It shows a transition to the intermediate skeletal structure in which the number of contacts that transmit large contact force of large particles increases as content of large particles increases. This indicates that the number of contacts that transmit small contact force of small particles has increased.

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Failure Analysis of Unsaturated Soil using Semi-Implicit MPM

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Key Words: *Unsaturated Soil, Failure Analysis, Material Point Method*

Water infiltration induces many natural hazards, e.g. slope failures, landslides and embarkment collapses. In particular, torrential rains have recently become more intense than before probably due to climate change. To simulate such hazards, particle methods have recently become popular, and, among them, the solid-liquid coupled material point method (MPM) has accomplished a remarkable progress in the area of computational geomechanics. This particular MPM is separated two types: one for saturated soil and the other for unsaturated soil. Especially for the MPM for unsaturated soil, it is essential to represent the decrease in shear resistance of soil by the transition from unsaturated to saturated sates by infiltration.

However, in most of the coupled solid-liquid MPM algorithms for unsaturated soil [1], the liquid phase is assumed to be weakly compressible, and as results often cause pressure oscillation. Also, this assumption requires a high computational cost due to the large bulk modulus of water when explicit time integration is adopted. Although several scholars [2] have proposed semi-implicit MPMs, which are empowered by the fractional-step method to overcome this problem, and proved its effectiveness, few studies have so far been made at enhancing it to deal with failure of slopes with unsaturated soil.

In this study, we develop a semi-implicit MPM to properly express the mechanical behavior of unsaturated soil based on Biot's mixture theory. The new contribution of this study is the incorporation of the fractional-step method into the MPM to solve the pore water pressure implicitly, which improves the numerical stability and computational efficiency. Several numerical examples are presented to demonstrate the capability and performance of the proposed method. In particular, a validation analysis is carried out using a model experiment of infiltration-induced landslide.

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Rheology of Segregated Bi-disperse Granular Flow in An Inclined Plane

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Key Words: Bi-disperse Granular Material, $\mu(I)$ Rheology, Size Segregation, Discrete Element Method

Size segregation is commonly observed in granular systems when the difference of component sizes is sufficiently large [1]. The bi-disperse granular system is the simplest system to investigate this phenomenon. In some previous contributions, it was found that the rheological properties of bi-disperse flows fall in the $\mu(I)$ rheology framework established for monodisperse ones [2], although the quantitative effect of segregation (different components) on flow mobility was not fully clarified [3][4].

In this work, we computationally explore the rheology of size-binary, steady dense flows on a slope using the two-dimensional discrete element method. A series of simulations are carried out for various assemblies of circular particles of identical total volume with different size ratios ($1.5 \leq S_r \leq 5.0$) and bulk volume fraction of large particles ($0.3 \leq V_r \leq 0.7$). The particles are randomly placed on an inclined rough plane ($17^\circ \leq \theta \leq 25^\circ$) with a periodic boundary setting in the streamwise direction and are let flow under the gravitational force until they reach a steady condition where the depth profile of the flow velocity, stress components, volume fraction and large particle fraction (f^L) is regarded as constant with some fluctuations. Then we take a time average of such variables for different depths to investigate their correlation in the framework of the $\mu(I)$ rheology model.

Our results show that (1) the bulk shear friction ($\mu = \tau/\sigma$) and the particle fraction ϕ are roughly but not perfectly described in $\mu(I)$ rheology model by using the generalized inertial number (I) proposed by [3], where the representative particle size is defined by the volume average of the large and the small particles size, where similar results were also reported in [5], (2) the deviation of the observed results is mainly caused by the shear friction and the particle fraction at the quasi-static limit (μ_0 and ϕ_0, respectively) to be a function of f^L. Based on the second result, we modeled the functions $\mu_0(f^L)$ and $\phi_0(f^L)$, which gives better predictions of μ and ϕ.

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Simulation of Bearing Capacity of Pile in Crushable Soil

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Crushable soils such as volcanic soils, carbonate sand or decomposed granites whose grains are easily break under foundation pressure, especially, large magnitude of stresses under pile tips. When the grains are crushed, particle size distribution (PSD) varies followed by higher compressibility of these soils. Pile foundation's settlement in crushable soils tends to be increased. Nonetheless, design code for bearing capacity of pile in crushable soil is still unavailable leading to a lot of difficulties for engineers to have an appropriate foundation design. This paper introduces a constitutive model for soils which takes account of the breakage mechanics including the evolutions of PSD and the compressibility due to grain crushing. The model is implemented in a finite element code to simulate a past experiment of pile penetration in crushable soil. Finally, parametric studies are carried out to investigate bearing capacity of piles in crushable soil.

Key Words: *Bearing capacity, Simulation, Crushable soil, Pile*

Simulations of Earthquake-induced Landslides by MPM

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Key Words: *MPM, Elasto-plasticity, Sediment flow, Landslide, Transition between solid and fluid, Actual terrain model*

In the last two or three decades, there has been consecutive interest in numerical simulation of damage caused by slope disaster such as landslides and mudslides triggered by earthquakes. It is, however, difficult to represent the collapse and subsequent sediment flow that are transitioned from the elasto-plastic and/or damage behavior of soil. To predict such a transitional behavior between solid and fluid states of soil, a single constitutive model for either solid or fluid is inappropriate and multiple models representing individual states should be properly combined.

To tackle this issue, we explore the novel constitutive model capable of representing the transition between solid and fluid states and discuss its applicability to the analysis of sediment flow induced by earthquakes using an elaborate terrain model. The model is formulated by the combined use of the Jaumann velocity-based hypoelastic-plasitc constitutive law of Dunatunga et al. [1], which is equipped with the μ-rheological model for granular flow proposed by Jop et al[2], and the standard Newtonean viscous model, and is implemented into the material point method (MPM). The resulting analysis tool has a capability to simulate collapse of soil structures and a sediment flow stemming from and ceasing at sedimented states.

After the basic performance of the proposed constitutive model is validated, several numerical examples are presented to demonstrate the capability in reproducing the transitional behavior from/to the sedimented state to/from the sediment flow. Also, to clarify the mechanism of sediment flow under the influence of seismic force and predict the subsequent sedimented state, we conduct a simulation of the landslide in the grounds of the Ebisu Circuit, which was caused by the Fukushima earthquake on February 13, 2021 using an actual terrain model with the detailed 0.5 meter topography data.

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Simulations of submarine landslide-induced tsunamis

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Key Words: *MPM, FEM, 3D-2D hybrid, Submarine landslide, Tsunami*

Submarine or/and subaerial landslides sometimes cause a series of hazardous events, such as the severing of submarine cables and pipelines, obstacles obstructing the operation of resource development facilities, and large-scale tsunamis. The damage caused by such a tsunami has been considered globally, and the loss of life has also been significant. However, the process of such an event is not well understood partly due to multiple physical phenomena simultaneously interacting (the collapse of the seabed, the interaction between soil and water). Conventional approaches make it difficult to predict the behaviours of soil and seawater with high accuracy. Therefore, it is necessary to develop novel numerical methods to evaluate the complex interaction between solid and liquid. For this purpose, we have proposed an MPM-FEM hybrid method [1] for expressing the complex interaction between solid and liquid, in which the MPM [2] is applied to the governing equation of the solid phase by the Lagrangian description, whereas the stabilized FEM [3] is applied to that of the liquid phase in the Eulerian frame. Since several numerical examples have demonstrated performance and capability of our proposed method, we will apply it to reproduce natural disaster on a large scale in this study. The tsunamis induced by submarine landslides that happened in Palu Bay, Sulawesi Island, Indonesia, in 2018 are our first target to simulate. However, using complete 3D computations to simulate the propagation of offshore waves require high computational costs and not suitable for large-scale and long-duration simulations. In this context, the 2D shallow-water equation has been widely used for simulating large-scale offshore wave propagation [4] because of its lower computational costs compared to full 3D computation. Since 2D approach is preferable in this respect, we will also develop a novel scheme that can couple with 3D and 2D domains for reproducing the whole process of tsunami induced by submarine landslides. The results of this study will help elucidate the mechanism of landslide-triggered tsunamis and are expected to contribute to the development of effective strategies for disaster prevention and mitigation.

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15th World Congress on Computational Mechanics (WCCM-XV)
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The effect of particle shape on rockfall events

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Key Words: DEM, rockfall, polygonal particles, shape effects

Rockfall events are a gravity-driven mass movements with limited volume but high energy and mobility. They are a significant hazard in mountainous regions and along engineered slopes with substantial potential for destruction (e.g. [1]). Mitigation of rockfall damage requires accurate prediction of potential rockfall trajectories and motion behavior. While various simulation methods have been proposed over the years, the common approach in discrete element simulations is to use round particles, see e.g. [2]. However, as real particles in rockfall events are rarely round but often angular and sharp-edged, round particle methods cannot accurately describe rockfall events. The dynamics of rigid bodies are heavily affected by the shape of the bodies as a competition of sliding, rolling, and even bouncing. Only recently have simulations begun to consider polygonal or polyhedral particles, e.g. [3], but they are still limited to a coarse selection of particle shapes. Up to now, no systematic study on the effect of particle shape in rockfall events has been performed.

With this research, we want to address this shortcoming by investigating the dependency of the motion behavior and runout distance of polygonal particles on the corner number and elongation for different initial orientations and slope angles using a two-dimensional discrete element method based on [4].

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Using 3D MPM to simulate multi phase gravity-driven mass flows for assessing the damage potential of cascading natural hazards

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Key Words: 3D MPM, multi-phase and multi material flows, gravity-driven mass movements, cascading natural hazards

Gravity-driven geophysical flows such as rock, ice and snow avalanches impacting large bodies of water bear the risk of causing cascading natural hazards. Such cascading hazards may include rock or snow avalanches followed by lake outburst floods. To evaluate the resilience of existing protection measures and to define adaptation strategies for the future, it is necessary to have instruments to asses the danger potential of such events. However, the numerical modelling of process chains is a challenging task, as multiple materials with differing properties and phases are interacting in the process. During such events, diverse physical processes such as fracturing and multi-phase mixing or impact, for instance with water, are common. In state-of-the-art operational models, these processes are usually not considered due to difficulties in their mathematical formulation and in the assessment of the respective parameters.
In order to address the challenges of simulating complex cascading processes of gravity-driven mass movements, we use a newly developed numerical model [1, 2] based on the 3D Material Point Method (MPM) and finite-strain elastoplasticity theory. Using this MPM framework, we analyse the flow of rock and snow avalanches in complex terrain and their interaction with mountain lakes by performing fully three dimensional simulations. As a case study, we present preliminary results of simulations of the "Salezer" snow avalanche in Davos, Switzerland. At this site, a snow avalanche was artificially released on January 15th 2019, impacting Lake Davos. In our simulations we use the snow conditions present on that day and the original release area mapped by a photogrammetric drone survey. We compare macroscopic flow features, e.g. the runout and deposition, of the simulated avalanche to the observations of this well-documented event. Furthermore, using different snow conditions and release areas, we identify critical scenarios endangering the infrastructure, touristic sites or inhabited areas in the vicinity of the avalanche track and the lake.

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Validation of DEM using macroscopic stress-strain behavior and microscopic particle motion in sheared granular assemblies

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Key Words: *Biaxial shearing, granular material, microscopic mechanism, particle rotation, numerical simulation*

Validation and/or calibration of distinct element method (DEM) models is usually performed by comparing element test simulation results with the corresponding stress-strain relationships observed in the laboratory [1]. However, such validation procedure performed at the macroscopic level does not ensure capturing the microscopic particle-level motion [2]. Thus, the reliability of DEM model may be limited to some stress paths and may not hold when the material response becomes non uniform for example when shear bands develop. In this study the validity of the DEM is assessed by comparing numerical result with experimental data considering both particle-scale behavior (including particle rotations) and macroscopic stress-strain characteristics observed in shearing tests on granular media. Biaxial shearing tests were conducted on bi-disperse granular assemblies composed of around 2700 circular particles under different confining pressures. Particle-level motions were detected by a novel image analysis technique. Particle rotations are observed to be a key mechanism of the deformation of granular materials. The results from this study suggest that to properly calibrate DEM models able to capture the mechanical behavior in a more realistic way particle scale motions observed in laboratory experiments along with macroscopic response are necessary.

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Computed tomography-based modelling of moisture-induced mechanical behaviour of sawn timber during kiln drying

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Key Words: *experimental validation*, *finite element method, transient, nonlinear, visco-elastic, hygro-mechanical, conditioning regime, dry density, Norway spruce*

Mathematical models play an important role in understanding drying processes in sawn timber and in the development of new drying schedules for kiln (i.e. air-circulation) drying of timber[1]. An experimental validation of such models is essential for their use in commercial applications. X-ray computed tomography (CT) is a non-destructive measurement method, which, in combination with suitable image-processing algorithms, allows for the reconstruction of the wood's fibre orientation[2], the observation of moisture content changes in wood during drying[3], and quantification of the deformations also experienced by wood during drying. Swedish sawmills use drying schedules for air-circulation drying that consist sequentially of heating, capillary, transition, diffusion, conditioning, and cooling regimes. The aim of the current study was to perform an experimental validation of a recently developed three-dimensional numerical model[4] based on moisture content and deflection data obtained through X-ray CT[5] and an image-processing algorithm[3]. The numerical model consists of two individual models that are determined in sequence: a moisture transport model based on a single-Fickian approach and a model that can simulate the visco-elastic and hygro-mechanical behaviour of wood. The experimental validation of the numerical model was determined using CT-data obtained during the kiln drying of a piece of sawn timber using a drying schedule provided by a local sawmill in the north of Sweden. The validation considered the transition, diffusion, and conditioning regimes since these are associated with moisture diffusion in wood. The objective of the study was to use the CT-data not only in the experimental validation, but also in the development of the model's geometry, the reconstruction of the fibre orientation, pith detection, and the definition of the simulation's initial states, boundary condition and moisture, temperature, and dry-density dependent material parameters. The validated model was used to analyze the effect of the conditioning regime on the moisture content and tangential stress development within the timber's cross section.

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Investigation of Chemical Elements Influence on Tracheid Effect by ICP-MS

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Key Words: *Tracheid Effect, Sapwood, Heartwood, Chemical Elements, Inductively Coupled Plasma Mass Spectrometry (ICP-MS)*

Tracheids provide not only structural support but also transport water as well as inorganic salts for the wood, in particular, the conifer. The direction of tracheid determines the direction of the fiber. To measure the direction of the fiber, tracheid effect was used to measure the in-plane angle, α, and diving angle on the wood surface. Both α and β were determined by the elliptical shape of a laser speckle dot [1]. Based on the tracheid effect, the three-dimensional fiber orientation scanning system (3D FOSS) was developed in the Photomechanics Laboratory at National Tsing Hua University (NTHU), Taiwan [2] . Images of laser speckle on sapwood and heartwood can be obtained respectively. It is possible to predict the modulus of elasticity (MOE) of the wood by employing the values of α and β. By comparing the predicted and material testing results of the MOE of the Japanese cedar, the tracheid effect was found being influenced by density, crack, roughness, etc.

Based on experimental investigation performed at NTHU, it was observed that different shapes of laser speckle of sapwood and heartwood were not caused by the diving angle. This observation was confirmed by using the scanning electron microscope. The difference of laser speckle shape may be possibly caused by organic or inorganic compound in cell wall or lumen of the tracheid. Therefore, in this paper, inductively coupled plasma mass spectrometry (ICP-MS) was employed to measure inorganic compound in sapwood and heartwood of Japanese cedar. By using the ICP-MS, samples are injected and lead to a plasma source to become ionized and analyzed. Hence, the ICP-MS has excellent selectivity and sensitivity as well as high accuracy. Content ratio and type of inorganic material can also be rapidly detected by the ICP-MS. Therefore, the ICP-MS is an effective method to observe distribution differences and trends of chemical elements between sapwood and heartwood.

The preliminary results obtained at NTHU show that the content ratio of inorganic material trend of potassium and magnesium between sapwood and heartwood of the Japanese cedar have high correlation. Therefore, characteristics of heartwood of Japanese cedar have strong relationship with the potassium and magnesium. Further results will be reported in the Congress.

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Long-Term Hygromechanical Behavior of Wood Exposed to Changing Climatic Conditions

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Key Words: *wood, moisture transport, moisture induced stresses, moisture induced failure*

Wood and wood-based products exhibit a strongly moisture-dependent behavior. Thus, knowledge about the wood moisture condition in a timber component is essential to predict its mechanical behavior during its service life. Not only stiffness and strength properties are highly dependent on the wood moisture content but also diffusion coefficients, density, specific heat capacity and the thermal conductivity. In addition, wood interacts with the surrounding climate, resulting in dimensional changes and stresses which may lead to critical conditions due to deformation caused by the non-uniform expansion coefficients. Therefore, modern prediction tools, which are able to describe these effects, can be of great benefit for the development of new wood-based products. Especially if these products exhibit complex geometries and are made of materials with different moisture characteristics. Such products have to be tested in varying climate conditions. Transport mechanisms below the fiber saturation point were described by Fortino et al. [1]. Three coupled differential equations describe bound water, water vapor and energy conservation. Free water exists above the fiber saturation point with the corresponding transport mechanisms described in Perre and Turner [2]. Values of the free water content can be much higher than those of bound water and water vapor. Thus, within the areas, where the switch from the transport mechanisms below the fiber saturation point to those above occur, high gradients can exist. To deal with these high gradients in terms of the finite element method different procedures like upstreaming and mass lumping described in Eriksson [3] were used. A three-dimensional Abaqus User Element Subroutine was developed to describe these coupled equations [4]. Such realistic moisture calculations allow in a next step to also conduct stress calculations. In combination with a multi-surface failure criterion for wood [5,6], it is then possible to evaluate the exposure of wooden structures to realistic climate conditions, taking into account the long-term material behavior as for example described in [7].

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Methods in an open-source framework for non-linear time-history dynamic analyses of Cross Laminated Timber structures subjected to Computational Fluid Dynamics wind actions

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Key Words: *Instructions, Multiphysics Problems, Industrial Applications, Covid-19*

Within the category of structures that show excellent seismic resistance performance, Cross Laminate Timber (CLT) is becoming more and more popular, also for its environmental compatibility qualities. The general tendency of this construction technology is to approach strategic and high-rise structures; these two tendencies are accompanied by the consideration of design methods for these structures that take into account the concept of resilience and performance-based design. The aim of this study is to contribute to the definition of methods and procedures for the advanced dynamic evaluation of these structures, with particular reference to the forces induced by the wind, which is currently a dimensioning element, above all to ensure sufficient comfort for the users of the structures.A novel modelling approach of CLT structures is proposed here that considers each single connector and the complex system of frictional contacts established in the various panel-to-panel joints , of the entire building. The simulation integrates the following modelling choices:

1. Structural panels are represented individually as shell elements with topological references of the intersections with the panels they are in contact with.
2. Panel-to-panel contact behavior is defined with a continuous frictional contact formulation
3. Connectors such as hold-downs and angle brackets are modelled as discrete elements
4. Distributed connections such as screws between vertical walls are represented by suitably calibrated shells
5. Calibrated Shell elements represent the behavior perpendicular to the grain of floor panels between two walls.

The validation of this method is carried out starting from the experimental test data of a full-scale 3-storey CLT structure, a campaign that was part of the CNR-IVALSA- SOFIE Project. In this case, the low-amplitude seismic tests are considered, in order to exclude plasticization of the connectors, and to directly compare the time-histories of inter-storey drift and base shear with the computational results. A support structure representing the wind-loaded envelope is then defined and the pressure field on it is calculated using Computational Fluid Dynamics (CFD) analysis. The development of a parser for these fields allows their subsequent use within a structural fem solver and their integration in a non-linear dynamic transient analysis.The software used are opensource allowing complete transparency of the methods used, the verifiability and improvability of the routines and the possibility for anyone to implement the methods discussed here.

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Modeling approach to estimate the bending strength and height effect of glued laminated timber beams

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Key Words: *Glued laminated timber, XFEM, Bending strength, Height effect, Failure mechanisms*

Numerical simulations provide a highly efficient way to estimate the bending strength of glued laminated timber (GLT) beams. A reliable estimation of the strength requires the consideration of adequate material behavior and relevant failure mechanisms.

Therefore, the approach uses section-wise constant material properties, i.e., longitudinal stiffness and tensile strength, which were derived along entire timber boards based on the procedure proposed by [1]. [2] proposed the use of discrete cracks without predefined positions within the framework of the extended finite element method (XFEM). Additionally, the formation of progressive crack networks is enabled by implementing cohesive surfaces between adjacent lamellas. For the validation, four-point bending tests of GLT beams were simulated to estimate the bending strength of specific beams from an experimental study with well-known knot morphology, which was presented by [3].

Finally, the height effect on the bending strength was studied by simulating GLT beam sections loaded with a constant bending moment. The beam heights ranged from 135 mm to 3000 mm, and the boards were randomly arranged within the GLT beams. As a result, we obtained fitted probability distributions of the bending strength for different global failure criteria and beam heights.

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Multi-Physical Modeling and Numerical Simulation of Thermo-Hygro-Mechanical Treatment of Wood for Use in Timber Structures

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Key Words: *Multi-Physical Constitutive Modelling, Thermo-Hygro-Mechanical Wood Treatment, Structural Investigations at Moulded Wooden Tubes*

The contribution at hand introduces computational modelling and realistic simulation concepts for a comprehensive description of the manufacturing and application of densified wood as well as densified and moulded wooden structures.

Wood, as a natural material, is characterized by a very good mechanical load-bearing capacity related to its density. Nevertheless, the ratio between its mechanical properties and its density can be optimized by densification technology for an improved use of wood in structural engineering. The wood densification process is not only a mechanical process with large and irreversible deformations, it is also characterized by temperature and moisture-dependent treatment of the wooden specimens.

Thus, the introduced approaches to predict the material and structural characteristics of compressed and moulded wood, consist of an inelastic and multi-physical constitutive modelling of wood at finite deformations, based on [1]. Furthermore, a computational approach to compute effective structural properties of wood after the thermo-hygro-mechanical densification process is introduced and presented, based on [2].

A successful implementation of the modelling concepts into the Finite-Element-Method (FEM) is presented, which is verified by numerical investigations. A validation of the numerical results is carried out by use of experimental data at beech wood (Fagus Sylvatica, L.). First, thermo-hygro-mechanical densification processes are modelled, see [3]. Second, the computed effective properties of densified beech wood are validated at experimental data. Finally, the structural investigations of densified and moulded wooden tubes with respect to their load deflection behaviour are presented. Therefore, digital image correlation based deformation patterns are compared to FEM based simulated deformation patterns for tubes under compressive loads.

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Phase Field Method-based Modeling of Fracture in Wood

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Key Words: *Wood, Phase field, Fracture*

Wood, as a naturally grown material, exhibits an inhomogeneous material structure as well as a quite complex material behavior. For these reasons, the mechanical modelling of fracture processes in wood is a challenging task and requires a careful selection of numerical methods. Promising approaches like limit analysis [1] or the extended finite element method (XFEM) in combination with microstructure materials models [2] deliver good but not yet satisfying results. Particularly the latter approach, including XFEM, has severe difficulties with crack paths in regions with complex morphology, mainly around knots. Therefore, in this work, focus is laid on the recently emerging and very popular phase field method [3]. Especially geometric compatibility issues that limit the use of XFEM can be avoided, as the crack is not discretely modeled but smeared over multiple elements. This allows the formation of complex crack patterns, defined by the underlying differential equations and boundary conditions but not restricted by the mesh geometry.

The present implementation contains a stress-based split [4] which allows proper decomposition of the strain energy density for orthotropic materials. Furthermore, the geometric influence of the wood microstructure on crack propagation is taken into account by a structural tensor scaling the length scale parameter of the phase field [5]. For solving the system of differential equations, a staggered approach is used where the phase field equation and deformation problem are solved separately. The staggered approach is enhanced with an additional Newton-Raphson loop that ensures convergence.

The developed algorithm was tested on various problems. Compared to XFEM more computation time was needed as the phase field method requires a finer discretization. However, crack patterns, including branching and merging, could be modeled very stable and accurately, even in the vicinity of knots where the material structure of wood is particularly complex and interface zones exist.

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Simulation of the temperature distribution in glued butt-joint timber connections

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Key Words: *numerical simulation, transient thermal analysis, Ansys, experimental validation, CLT, glued butt-joint*

With the Timber Structures 3.0 technology, timber components are bonded together in a statically load-bearing manner by a 4 mm thick butt joint on the face side of cross-laminated timber (CLT) plates filled with a casting resin. In particular, this offers the possibility of creating biaxial load-bearing ceiling panels made of CLT in any geometry.

However, the processing temperature of at least 17 °C [1] specified by the casting resin manufacturer still poses a challenge for the construction site application. Therefore, the possibility of locally tempering the 4 mm thick casting resin joint during the curing process is being investigated. For this purpose, a groove is milled into the surface to be cast, into which a heating wire is inserted. This heating wire is intended to heat the casting resin joint to above 17 °C during curing by low ambient temperatures.

In order to investigate whether this measure causes a sufficient temperature in the joint, a numerical simulation is carried out in Ansys. For the timber, the material parameters (thermal conductivity and heat storage capacity) are known as a function of the respective fibre direction, but for the casting resin, the values known for the cured state are used first. Although these differ from those in the fluid respectively curing state, they represent a good first approximation. Likewise, a justified assumption is made for the exotherm. With these input values and clearly defined boundary conditions of geometry, ambient temperature and heat transport, the temperature distribution in the joint is calculated over time and over the cross-section. Subsequently, an experiment with the same boundary conditions is carried out and the results are compared. In the following, the material parameters of the casting resin in the simulation are adjusted so that the simulation and experiment match. With the values determined, the application is planned and carried out on the construction site.

To verify the input values, the site application is monitored with temperature sensors and compared with the previous simulation. This comparison shows that the simulation represents reality sufficiently accurately. Therefore, the simulation can be extended to different boundary conditions, such as panel thicknesses and ambient temperatures, and used in the future to determine the number and amperage of heating wires for construction projects at below 17 °C.

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Wood-Water Relation Revisited from Molecular Scale

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Key Words: *Molecular Simulation, Cell Wall, Interface, Wood-Water Relation, Hygromechanics*

Wood cell wall, especially the thickest S2 layer, dominates the hygro-mechanical performance of wood. The exploitation of the full potential of wood calls for a thorough understanding of its mechanics and hierarchical structure, especially of the nanoscale wood-water relation.

The exact material configuration of cell wall is still under debate because the nanoscopic polymer interactions are beyond the detection limits of contemporary experimental techniques. In contrast, computational studies, especially molecular modelling methods, are capable of agilely experimenting various material configurations and probing the working water-wood mechanisms on the molecular scale.

We employ molecular dynamics (MD) simulations to understand the structural, physical, and mechanical impact of hydration on wood cell wall. Individual polymeric components, their composites and interfaces, and a state-of-the-art S2 cell wall layer model are proposed and characterized systematically. The yielded unprecedented micromechanical dataset reveals the working mechanism of cell wall that is otherwise unobtainable.

It is demonstrated that the interphases between different polymeric components exhibit densities or mechanical properties distinct from bulk material. Although the matrix itself is soft and isotropic in bulk, its interphase is stiff and anisotropic owing to the influence of cellulose fiber. Hydration induces the weakening of wood cell wall by causing mechanical degradation of matrix and fiber-matrix interface while leaving the cellulose fiber mostly intact. Hemicellulose glues lignin and cellulose fiber together, and water severely disturbs the hemicellulose-related hydrogen-bonds. In contrast, lignin is rather hydration independent and serves mainly as a space filler. The fibril-fibril and fibril-matrix interfaces are probed by MD pulling tests. The stick-slip behavior is explained by the strong correlation between the number of hydrogen bonds and the interfacial shear stress, suggesting the force rendered by a single hydrogen bond to be ∼140 pN.

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A finite element analysis of expansive bedrock considering electro-chemo-mechanical coupling phenomena in crystal layers of clay minerals and degradation of the internal structure

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Key Words: *expansive clay mineral, electro-chemo-mechanical phenomena, cementation, tunnel, finite element method*

In bedrock including expansive clay minerals, the pore fluid composition affects the mechanical behavior of the bedrock such as swelling. It is necessary to elucidate the mechanism of the behavior and evaluate the deformation caused by the swelling quantitively because the swelling behavior of expansive bedrock causes problems when tunnel excavation and earth cutting. To simulate the issues regarding swelling behavior, a constitutive model that considers the electro-chemo-mechanical phenomena on the surface of expansive clay mineral crystal, stiffness of bedrock, and the degradation of the internal structure is required.

This research proposes a new model targeting expansive bedrock by means of combining an elastoplastic model considering electro-chemo-mechanical phenomena with the Cam-clay model introducing cementation and its degradation due to plastic deformation. The proposed model describes the process of degradation of cementation due to the swelling caused by the electro-chemo-mechanical interlaminar action occurring between crystal layers, which can lead to the transition of a rigid rock mass to soft soil.

Tunnel excavation and swelling analyses are demonstrated by incorporating the proposed model into a finite element analysis code. The simulation results indicate that the proposed model is applicable to the geotechnical problems occurring in expansive bedrock.

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A numerical Simulation of CPT Test Based on a Cavity Expansion Theory by Using Effective Stress Analysis

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Key Words: *FEM; effective stress analysis; penetration; model test; cavity expansion*

Although the penetration resistance is not a physical parameter inherent to the soil material but is a value reflecting the response from the ground, there are many estimations that directly associate penetration resistance with various ground physical properties. Penetration resistance is subject to both the influence of the properties of the ground material such as strength parameters or dilatancy of the soil, and the influence of the boundary condition such as layer boundary and drainage condition around the target ground. Therefore, in order to improve the accuracy of the CPT, it is im-portant to analyze the behavior of the soil by considering cone penetration as a complicated boundary value problem and clarify the influence of boundary conditions and soil characteristics on penetration resistance.

As preparation for a future numerical investigation focused on the details of the combined effects of soil properties and various boundary conditions, a series of numerical analyses was conducted using a FEM code named GEOASIA (All Soils All States All Round Geo-analysis Integration) developed by Asaoka et al. in [1] and sophisticated by Noda et al. in [2], in which the Super/subloading Yield Surface Cam-clay model, in short, the SYS Cam-clay model in [3,4] was used as the constitutive equation of the soil skeleton.

The influence of mesh size on the tip resistance is confirmed at first. Then, as a part of preparations for future experimental validations through numerical simulations of a series of calibration chamber tests, a series of numerical parametric simulations evaluating the influence of lateral boundary conditions and confining pressure on cone tip resistances are conducted. Further, the analytical results are roughly compared with a series of trial experimental results. Since those experimental results contained some ununiformity problem of stress distributions in the model ground, it remained that a similar qualitative tendency was observed between the simulation results and the experimental results.

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A slope stability analysis over a large area using Hovland's method and three-dimensional simplified Bishop's method

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Key Words: Slope stability analysis, Hovland's method, Three-dimensional simplified Bishop's method

Hovland's method[1] is well known as one of the three-dimensional limit equilibrium methods for slope stability analysis. The method has been widely employed even in practical situations because of its simple calculation algorithm, while a lot of researchers have pointed out that the method cannot accurately evaluate the risk of slope failure. On the other hand, more sophisticated methods, such as simplified Bishop's method[2], simplified Janbu method[2], and Spencer's method[2], are also recognized as methods based on the limit equilibrium theory. Although calculation algorithm of these methods are much complex than that of Hovland's method, the importance of using those methods has been mentioned in a lot of literatures. However, the potential of the methods has been discussed only under limited conditions and the capability of each method for risk analysis of wide-area disasters has not been well studied.
This study aims to explore the accuracies of Hovland's method and simplified Bishop's method by applying them to wide-area slope stability analysis under the condition of a real heavy rainfall event. In order to consider realistic slip surface, both methods are extended to satisfy the moment balance under the assumption of the ellipsoidal slip surface. However, since Hovland's method is generally formulated under the assumption of circular slip surface, the original Hovland's method is also used for comparison. Slope stability analysis are then performed using these three methods to reproduce the slope failures caused by an actual heavy rainfall event. Distribution maps of the factor of safety are compared with the actual slope failure distribution and the consistency is quantitatively compared using the ROC curve. The obtained results indicates that the result obtained by simplified Bishop's method is the most consistent with actual slope failures.

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Coupled Bond-Based Peridynamics and DEM with Softening Model for Cracking and Failure of Compacted Clay

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Key Words: *Peridynamics, DEM, Geotechnical engineering, Fracture mechanics*

Peridynamics is characterized as a continuum-based, mesh-free, and non-local numerical analysis method. Many studies have shown that the peridynamics is one of the effective tools for crack propagation and fracture phenomena in brittle and quasi-brittle materials. In the field of civil engineering, the peridynamics has been successfully applied to the problems of the fracture of rocks and concrete structures. Compared to these types of materials, there are a few applications to the problem of the fracture of soils, such as mudstone and compacted clay [1]. The soils are quite different from the rocks and the concrete in that they need to be observed after cracking and failure. For the soils, it is necessary to deal with both the fracture and the post-fracture, while for the rocks and the concrete, it is sufficient to deal only with the fracture.

The study proposed a 3-D combined model of the peridynamics and the DEM (Discrete Element Method) to continuously handle the process of the failure of the compacted clay [2]. The bond-based model of the peridynamics is employed to reproduce the behavior from the initiation of cracks to the fracture. At the same time, the DEM is also introduced so that the interaction forces between the fragmented pieces after the fracture can be calculated including the friction force. In addition, a bilinear bond softening model was introduced to obtain a nonlinear stress-strain relationship which is often seen in the compacted clay. The proposed model was validated by comparing the experimental results and the numerical results of the uniaxial compression test and the diametral compression test of the soil specimens with a single initial crack.

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Development of a stability analysis method of reinfoced soil by hybrid type rigid-plastic finite element method

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Key Words: *Rigid-plastic finite element method, Soil reinforcement, Anisotropic strength, Soil-reinforcement interaction, Duality*

The authors developed a hybrid type rigid-plastic finite element method (RPFEM) [1] for a stability problem of the ground. This method is based on the Lagrangian function of lower bound analysis with spatial discretization of the finite elements. Due the the duality of limit theorems, both stress and velocity fields can be solved simultanesouly by the interior point method of Second cone optimzation programming. In this study, a simple model of the interactions of reinforcement members and the surrounding ground is proposed and implemented into RPFEM to evaluate a stability of a reinforced ground.

A bearing capacity mechanism of a ground reinforcement method is a confining effect of soils by the reinforcement members, i.e., confining forces or pressures by the reinforcement members enhance the resistance against failure. In order to deal with a reinforced ground problem in the framework of RPFEM, Asaoka et al. [2] added velocity constraints between two nodes, such as no change in lengths or angles to the upper bound limit analysis . From the point of the duality of limit thoerems, these velocity constraints stand for unlimited strengths of the reinforcements.

In the formulation of hybrid type RPFEM, both velocities and stresses are unknow variables. Considering the duality, velocity constraints are always accompanies by Lagrangian multipliers, which can be interpreted as confining forces. So, we can simply introduce inequality constraint conditions on these confining forces to express limited strengths of reinforcement members. This is a direct extension of the previous study [2], but this extention can be only achieved by the hybrid type formulation of RPFEM.

Velocity constraint conditions are imposed on the nodes of a finite element of a ground. Only a mesh of a ground is required. No special finite elements are required for reinforcement members. In addition, slipage between reinforcement members and the surrounding ground can be modeled by introducing inequality constraints of two adjacent member forces. This model is similar to an interaction between piles and soils, i.e., a change of axial forces of piles at two sections due to skin frictions.

This newly proposed method can predict various failure modes including member-failure and pull-out failure as solutions without any assumption of failure modes. Some numerical examples are presented to demonstrate the features of the proposed method.

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Differences in Using Ceramic Discs and Microporous Membrane Filters for Suction Control in the Axis-Translation Technique for Unsaturated Soils

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Key Words: *Unsaturated Soil, Ceramic Disc, Microporous Membrane Filter, FEM Simulation*

Ceramic discs, which have high air entry values, are commonly used for matric suction control in the axis-translation technique for element tests on unsaturated soils. The main limitation of this method is the long duration time of unsaturated element tests due to the low permeability of a ceramic disc. As an alternative, microporous membrane (MM) filters have been introduced to shorten the necessary time for establishing suction equilibrium. Nevertheless, some researchers pointed out that there are some discrepancies in test results when using ceramic discs and MM filters.

In this study, to investigate the differences between using ceramic discs and MM filters, triaxial tests on unsaturated completely decomposed granite, or called Masado in Japan, were firstly conducted using the two matric suction control methods. Then, soil-water-air coupled finite element analyses were conducted to simulate the consolidation process in triaxial tests as initial/boundary problems. In the numerical calculations, a saturated/unsaturated soil constitutive model and a water retention curve (WRC) model [1] were employed to describe the hydro-mechanical behaviors of unsaturated Masado. Meanwhile, the WRC and permeability-saturation relations of a ceramic disc and an MM filter, as porous materials, were properly taken into consideration.

Both the experimental and numerical results showed that the changes in degree of saturation and suction within the ceramic disc are no longer interpreted as element behaviors. In the numerical calculation, after applying suction to the specimen, though the ceramic disc remained highly saturated, the suction within it significantly increased, which resulted in the greater drainage discharge of the specimen. Therefore, the axis-translation technique in triaxial tests for unsaturated soil with ceramic discs should be reassessed as an initial/boundary problem.

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Dynamic coupled analysis with complete formulation of unsaturated soil in centrifuge tests

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Key Words: *complete formulation, relative acceleration, unsaturated soil, centrifuge test*

Dynamic coupled analyses considering pore air of unsaturated soil have been performed. Pore air plays an important role in the dynamic response of unsaturated soil and hence the pore air pressure should be explicitly considered in the formulation of dynamic problems. However relative acceleration of pore water and air to soil skeleton has been usually ignored in simplified formulations such as *u-p* formulation [1]. Complete formulations such as *u-U* formulation considering the relative acceleration of pore fluid [2] have been already presented; however, the effect of relative acceleration of pore fluid on seismic response of unsaturated soil has not been clarified. In dynamic centrifuge tests with saturated soil viscous water has been used as a pore fluid to reduce the permeability. However pure water has been used in some cases with unsaturated soil; therefore, the effect of relative acceleration can be significant.

In this study the effect of relative acceleration of pore fluid on seismic behaviour of unsaturated soil is discussed through numerical simulations with complete and simplified three-phase coupled formulations. First both formulations governing the dynamic behaviour of unsaturated soil, u-v-p and u-p formulations, were briefly shown based on porous media theory and constitutive models. Next both formulations were used for the simulations of dynamic centrifuge experiments with unsaturated embankment dam [3] and slope [4]. The effect of relative acceleration of pore fluid on seismic behaviour of unsaturated soil was discussed through simulations of centrifuge experiments.

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Evaluation of slopes subjected to intermittent rainfall conditions

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Key Words: *Slope failure, Intermittent rainfall, Unsaturated soil,*

Rainfall induced landslides are a quite common phenomena that happen all over the world consequential to climate change. Safety margins of these slopes possess high during the period of dry weather conditions with the help of unsaturated soil mass above the groundwater table. As a result of prolong rainfall conditions, destruction of matric suction causes triggering of slope failures. Many published data revealed that slopes experience mostly an intermittent rainfall conditions rather a steady rainfall before the failure took place. To investigate the slopes subjected to intermittent rainfall conditions, this study carries out a series of centrifuge tests. The generation of excess porewater pressure and deformation of slopes are recorded using pore-pressure transducers and image recording system respectively.

The aim of this paper is to compare and validate the physical modelling test results by numerical simulation. The unsaturated soil behaviour is simulated using the three-phase (soil-water-air) coupled hydro-mechanical model which is based on the governing equations derived by [1]. A conventional elastoplastic model and soil-water characteristic curve (SWCC) model are incorporated in these simulations. It is expected to demonstrates the ability of this model to evaluate the temporal variation of pore-pressure and the deformation process of slopes subjected to intermittent rainfall conditions.

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Hydrologic-geotechnical Modelling for Multihazard Analysis of Landslide and Flood caused by Heavy Rainfall

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Key Words: Surface Flow, Infiltration, Slope Stability, Shallow Landslide, Flood Inundation

Landslide and flooding are two of the most common hazards associated with intense and heavy rainfall. While the relationship and coexistence between the two hazards have been observed and documented, limited studies have been published assessing both hazards, with most studies focusing exclusively on either landslide or flooding. Therefore, this study presents a regional-scale multihazard approach characterizing the nature of both phenomena through a combination of hydrologic and geotechnical principles. This is done by incorporating surface flow, infiltration, and slope stability analyses to visualize the spatio-temporal response of both landslide and flooding with respect to intense or heavy rainfall.

To reduce computational costs, a hybird approach using local- and zero-inertia models [1] of the two dimensional shallow water equations is utilized to approximate the surface flow curbing restrictive time-step conditions common in hydrologic models. Moreover, rainfall infiltration is approximated using the one-dimensional Green-Ampt model [2], and slope stability is obtained using a limit equilibrium method defined for an infinite slope whose failure mechanism is generated from the forces arising from the effects of surface flow and the downward propagation of the wetting front [3]. The model is then applied in Marumori, Japan which suffered numerous landslide and flooding disasters during Typhoon Hagibis in 2019. Validation indicate that the proposed model successfully simulates the hydrologic and geotechnical response of slopes showing the distribution of both unstable slopes and inundated areas indicative of landslide and flooding hazards.

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Large Deformation Simulation for Geotechnical Engineering Based on Cosserat Continuum Theory and Isogeometric Analysis

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Key words: *Isogeometric Analysis, Finite Element Analysis, Strain Localization, Elastoplastic, Cosserat Continua, Saturated Porous Media, Biot Consolidation Theory, Shear Band*

Combined with the Cosserat continuum theory, the isogeometric analysis is extended to simulate the strain localization problems of geomaterials due to strain softening, that leading to the so-called Cos-IGA method. The numerical results demonstrate that the numerical solution based on Cos-IGA is convergent and mesh-independent and that the Cos-IGA has the ability to capture the initiation and propagation of shear band as strain localization problem involved. Also, it illustrates that the Cos-IGA effectively avoids the shortcomings of mesh distortion and overstiffness in Cos-FEA, and improves the path-bifurcation phenomenon and makes the transition of force-displacement curve smoother in softening stage due to the non-interpolation and variation diminishing properties of NURBS basis functions.

Also, the Biot-Cosserat continuum theory is combined with isogeometric analysis (Biot-CIGA) to simulate dynamic strain localization in saturated soils. The results demonstrate that Biot-CIGA can solve the ill-posed problem of saturated soils caused by strain-softening properties and non-associated flow rules, thereby obtaining a convergent, mesh-independent numerical solution. Compared with the finite element analysis of Biot-Cosserat continuum, the high-order continuity of Biot-CIGA provides a smooth pore pressure gradient field and thus ensures the local mass balance of pore fluids. Additionally, the Biot-CIGA describes the inflow and outflow of pore fluids in the element, which means it is able to accurately simulate the volumetric strain of the element. Simulation results also show that the Biot-CIGA method can also effectively alleviate the mesh distortion in shear bands when materials experience large deformation. Last but not least, because Biot-CIGA adopts NURBS as its shape functions, it can conduct simulations directly on CAD models, which not only maintains the precise geometry, but also avoids an expensive intermediate meshing step.

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Mathematical and numerical modelling of biomediated soil improvement

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Key Words: *MICP, electricity-reaction-diffusion system, homogenization method*

Soil improvement techniques have been developed experimentally and empirically from various geotechnical viewpoints based on physical, chemical, and biological findings. According to traditional microbiological perspectives, microbially induced soil cementation techniques have been attracted as an environmental-friendly soil improvement technique. Microbially induced carbonate precipitation called as MICP, especially, has been known that microbial metabolism can induce a precipitation of calcium carbonate in the pores and on the surface of sand particles. Eventually, the ground is stabilized physically since discrete sand particles can be bound by calcium carbonate.

The precipitation and growth of calcium carbonate on the sand surface and its pores can be simulated using the recently proposed numerical simulation techniques. However, these proposed techniques have not incorporated parameters such as electrical properties and adsorption. Therefore, the precipitation process on the sand surface and the bridging pattern between sand particles remain ambiguous.

In the current study, the authors proposed a novel multi-physical model that considers the behavior of microorganisms and ions in a weak electrostatic field around the sand particles. To validate the proposed model, lab-based MICP experiments were conducted, and the experimental and simulation results were compared. Furthermore, the changes in mechanical parameters due to calcium carbonate precipitation were investigated by integrating the homogenization method into the proposed model.

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Mathematical and numerical modelling of photoautotrophic calcification on rock surface

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Key Words: *Reaction-diffusion system, photoautotrophic microbes, calcification*

Traditional stabilization of weathered rock surfaces has relied on physical approaches such as anchoring and retaining walls. Naturally, these techniques require ongoing maintenance and restoration, as their effects are not permanent. Thus, the development of novel techniques of rock-surface stabilization with self-organizing and environmentally friendly restoration functions has been required.

On the other hand, microbially induced rock surface improvement techniques have attracted a great deal of attention in recent years. This technique enhances the mechanical properties of rock surfaces by precipitating calcium carbonate microbially. It is interesting to note that microbial protection techniques based on photoautotrophic microbes like green algae and diatoms would be helpful in protecting aging rock surfaces. Photoautotrophic calcification may achieve self-organizing restoration of aging rock surfaces since the microbes can grow and induce calcium carbonate precipitation under sunlight continuously. However, in most of traditional research, this novel technology has been studied by laboratory and field investigations, and has not been examined by mathematical and numerical approaches. This is because mathematical models for the analysis of the coupled behavior between microbes and calcification have not yet been proposed.

In this study, the authors propose a novel multi-physical model based on the reaction-diffusion system that considers the behavior of photoautotrophic microbes and the precipitation of calcium carbonate on rock surfaces. As a result of numerical simulations, it was clarified that the self-organizingly precipitation of calcium carbonate on rock surfaces can be expressed by the proposed model.

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Modelling landslide debris flow with entrainment: development and validation

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Key Words: *Landslide, debris flow, debris mobility modelling, entrainment*

The volume and mobility of a debris flow could increase with distance travelled as it has the potential to entrain a substantial amount of channel-bed material along its travel path. This entrainment effect renders the debris flow more devastating to downslope populations and facilities. In modern landslide risk management, being able to predict the characteristics of debris flows is essential for the design of mitigation measures against landslide hazards. Such need has led to the development of a variety of debris mobility models around the world in recent times. There is a need for modelling methods which are capable of simulating entrainment effects in a rational but practical manner.

Over the past two decades, the Geotechnical Engineering Office (GEO) of Hong Kong has expended considerable effort to develop debris mobility modelling tools for use in routine engineering practice for forward prediction purposes. Recently, GEO has completed a study to enhance an in-house debris mobility code. Physical parameters which can be estimated from the field by engineers or geologists are incorporated in the code to predict entrainment effects in a simple and rational manner. This allows the modelling of varying entrainment potential along a debris flow path. The code has been checked against simplified analytical solutions and validated against field observations in a major historical landslide event involving high-mobility debris flows in Hong Kong. The numerical modelling results indicated that simulated entrainment volume and mobility characteristics are broadly consistent with geological field mapping records.

Numerical elucidation of the graben crack damage that formed in the Aso caldera due to the 2016 Kumamoto earthquake

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Key Words: *Stratum irregularity, Soft clay, Consecutive earthquake, Seismic response analysis*

In the 2016 Kumamoto earthquake, graben crack damage occurred in the northwest part of Aso Caldera. It was thought that the Futagawa fault zone did not reach to the Aso Caldera, and no causal relationship has been identified between the graben damage and the fault zone. Therefore, various causes have been considered, such as collapse of underground cavities, surface seismic faults, liquefaction-induced horizontal movement in deeper ground, etc. However, the definite cause of graben cracks have not been identified yet. Yasuda et al. [1] revealed that most of the grabens appeared at the location above the old lake which existed about 9,000 years ago. In addition, they have confirmed that the lake sediments have the property that the shear rigidity decreased sharply with strong repeated shear stress from the laboratory testing.

The aim of this study is to elucidate the mechanism of graben cracks formed in the Aso Caldera in terms of "stratum irregularity" formed by the old lake basin in the Aso Caldera, the "presence of soft clayey soil" of the old lake deposit and the "two consecutive earthquakes" that characterize the Kumamoto earthquakes. Therefore, 2-dimensional seismic response analysis was conducted to elucidate these effects on the subsurface damage. The analysis code was the soil-water coupled finite deformation analysis [2], which incorporates an elasto-plastic constitutive model that allows description of mechanical behavior of soils ranging from sand through intermediate soils to clay within the same theoretical framework [3]. The following conclusions were obtained.

(1) By considering the effect of stratum irregularity, (a) the focal phenomena of the body waves, (b) the excitation of the surface waves and (c) these amplification interference ("edge effect") were numerically reproduced. Therefore, the wave propagation became intricated and the oscillation became larger at a specific point near the ground surface.
(2) The clayey lake deposit was in a soft condition. Therefore, the effective stress was easily decreased by seismic motions, which causes further increase in natural period of the ground.
(3) As mentioned in (2), natural period of the ground was increased by foreshock. The continuous occurrence of main shocks significantly amplified long-period oscillations. This long-period and large shaking caused graben damage at the surface.

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Numerical simulation of pile penetration into geomaterials using particle-element coupled method

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Key Words: *construction process analysis, particle-element coupled method, large deformation*

In the soil-structure interaction analysis, substructures installed in the ground are modelled where they are planned to be, ignoring their construction process. This type of numerical modelling is called *wish in place method*, which does not occur in actual construction sites. However, this type of numerical simulation is very popular in the practical engineering because it is quite simple to model the target system. The method has disadvantages, for example, that in case of simulating a driven pile penetration into geomaterials the method cannot consider the volume convection of geomaterials. The reason why the conventional numerical methods, e.g., FEM, have not considered for or they have not been applied limitedly to the construction process with the volume convection is because the discretized elements are not suitable for the large deformation, and because they need the intensive computational cost in re-meshing of the target system.

Particle-based method is one of the numerical methods of continua, giving a solution for simulating the construction process analysis. Particle-based method is capable of considering the volume convection of geomaterials and simulating the intensive large deformation. In this study, the authors have performed the numerical simulation of a pile penetration into geomaterials using the particle-element coupled method (PEM) [1], which is the combination of particle- and element-based method enabling the reduction of computational costs. According to the numerical results, PEM can simulate both the ground resistance and deformation with good agreements, and it also realized that the ground resistance and deformation are dependent on geomaterial dilatancy characteristics.

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Quantification of the effect of rock shape proparties on the distribution characteristics of rockfall run-out

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Key Words: *Rockfall, Distribution Characteristics, Rocky-DEM, Shape Effect, Sphericity*

This study aims to quantify the contributions of rock shape on the characteristics of rockfall run-out. A series of rockfall simulations is performed using the Discrete Element Method (DEM) to analyse the relationships between rock shapes and rockfall movements. A software Rocky-DEM, which is capable of handling polygonal elements, is employed[1] to conduct this numerical experiment.

In order to define rock models with different shapes, we vary the geometrical parameters that are aspect ratio, oblateness, and cut ratio. A total of 200 simulations are carried out for each of 36 different models characterized by these three parameters. Although the three parameters are used to control the shape properties, the parameters partially represent characteristics of rock shape, and there is some overlap in the physical meaning of these parameters. To overcome the problems, the sphericity, which is a measure of how close the object is to a sphere, is newly employed for analysing the contributions of rock shape. There have been however a lot of definitions of sphericity, we employ some of them to investigate the effectiveness of each sphericity. In terms of rockfall run-out, the mean and the coefficient of variation obtained from the distribution maps of the final run-out position are quantified to characterize the distribution characteristics. Based on the results of all calculation cases, the correlation between the statistical values of rockfall run-out and the sphericity is examined.

The obtained results show that two of the sphericities have a strong contribution on the distribution characteristics. According to a result of the principal component analysis, it was also found that the two sphericities have a mutually influence on the rockfall run-out. It is therefore concluded that it is possible to represent characteristics of rockfall run-out by the two sphericities.

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Reconstruction of isotropic Cam-clay model based on multiplicative decomposition of deformation gradient

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Key Words: *Cam-clay model, Elastoplastic analysis, Multiplicative decomposition of deformation gradient, zeta stress, Eshelby-zeta stress*

In the framework of finite deformation elastoplasticity, several researchers (e.g., Borja and Tamagnini, 1998; Yamakawa et al., 2010) have formulated the Cam-clay model that was based on the multiplicative decomposition of the deformation gradient and employed a hyperelastic body. However, these pioneering works do not fully consider the volume change in the intermediate configuration. This shortcoming makes the previous models unable to guarantee the existence of the state boundary surface, which plays an important role in the derivation of the Cam-clay model.

Therefore, this study reconstructs the isotropic Cam-clay model that can explain the existence of the state boundary surface using zeta stress and Eshelby-zeta stress derived by considering the non-negativeness of plastic dissipation by focusing on the unit volume in the intermediate configuration with referring to Bennett et al. (2016). In the proposed formulation, the hyperelastic body proposed by Houlsby et al. (2006) is applied to the elastic part. This study also constructs an implicit stress update algorithm for the model and derives the tangent modulus consistent with the algorithm. Moreover, to verify the reconstructed model and the stress update algorithm, numerical analysis is performed using finite element analysis code that implements the model.

By simulating triaxial compression tests to verify the model and algorithm, this study presents that the developed code can reproduce the basic mechanical behaviors of reconstituted and normally consolidation clay. In addition, the simulation also demonstrates that the derived implicit stress update algorithm and the consistent tangent bring the quadratic convergence to the global Newton-Raphson procedure for finding equilibrium of force.

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Seismic Response Analysis of Embankment Dams by Velocity-based Space-Time FEM

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Key Words: *Seismic response, Dam, Space-Time finite element method, Elasto-plastic constitutive model*

The safety of earthen structures, such as dams, tunnels and embankments, draws growing attention in Japan, which is one of the most earthquake-prone countries in the world. In order to assess the safety of the structures during earthquakes, the dynamic response analysis is numerically conducted commonly by the finite element method. In finite element framework, several methods have been proposed to achieve accurate results, and one of them is the velocity-based space-time finite element method, abbreviated by v-ST/FEM, which is based on time discontinuous Galerkin method.

The conventional method for the assessment of seismic performance of dams investigates the seismic response assuming the elastic behaviour of the structure, and predicts the permanent deformation caused by a slip surface having the lowest factor of safety according to the above seismic response analysis. However, this method results in the inaccurate prediction of both the seismic response and the permanent deformation especially when the structure is subjected to seismic loading induced by big earthquakes, called level-2 earthquakes. Then, the seismic response analysis in which appropriate elasto-plastic constitutive models are installed is required in order to predict the permanent or residual plastic deformation accurately.

Velocity-based space-time finite element method (v-ST/FEM) for the seismic response analysis of earth-fill or rock-fill dams, which undergo the permanent deformation during strong-motion earthquakes, is developed herein, assuming the infinitesimal deformation. Since the space-time FEM realizes the higher accuracy of time integration, the performance of v-ST/FEM is compared with that by Newmark-β through a one-dimensional problem, i.e., the propagation of a shock-wave. Then, two-dimensional seismic response analysis of existing rock-fill dams are carried out, in which an elasto-plastic constitutive model based on Mohr-Coulomb criterion is implemented in v-ST/FEM, and the permanent deformation of rock-fill dams are computed as well as the dynamic ground motion.

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Simulation of deformation followed by failure of unsaturated slope in a rainfall model test

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Key Words: *Soil-Water-Air Coupled Elastoplastic Finite Deformation Analysis, Unsaturated Soil, Inertia Force, Rainfall*

In recent years, there have been many collapses of slopes due to heavy rain. In most cases, to predict the collapses of slopes in heavy rainfall, seepage flow analysis and stability analysis are used together. However, it is insufficient to perform a stability analysis that judges whether a safety factor exceeds 1 or not, using the stress state determined from a seepage flow analysis. It is necessary to analyze slope behavior from deformation to failure caused by seepage. In addition, the failure phenomena are accompanied by acceleration motions even if the external force is rainfall. Therefore, it is necessary to take into consideration the inertial force. Furthermore, to simulate large deformation that leads to failure, it is essential to consider change in the geometry based on finite deformation theory.

With the above background in mind, a rainfall model test [1] was simulated using a soil-water-air coupled finite deformation analysis code considering inertia force [2] to elucidate the failure mechanism of unsaturated slope. The constitutive model for the soil skeleton is an elastoplastic constitutive model employing the unsaturated effect in the Super/subloading Yield Surface Cam-clay model (SYS Cam-clay model) [3,4].

As a result, we succeeded in simulating the rainfall-induced deformation behavior leading to failure accompanied by acceleration. The failure mechanism is explained as follows: 1) The entire unsaturated slope became a normally consolidated state caused by an increase in saturation degree (a decrease in suction), in addition to a rise in pore pressure and an increase of self-weight. 2) The stress state became located above the critical state line in mean skeleton stress p'–deviator stress q space especially near the slope toe where pore water gathered. Therefore, the soil element showed softening behavior with plastic volume expansion, which is a characteristic of the Cam-clay model. 3) A slip failure started to occur near the slope toe, and suddenly expanded to the upper part of slope with a significant acceleration.

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Simulation of Lateral Compression-induced Fault Topographies based on the Non-linear Elasto-plastic Soil Mechanics

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Key Words: *Thrust, Compression, Imbrication, Décollement, Elasto-plasticity, FEM*

Lateral compression of ground generates a wide variety of fault topography such as thrusts and décollements with a single displacement discontinuity. As for typical structures with multiple slip surfaces, there exist a "pop-up" with conjugate slip surfaces, and an "imbrication" with parallel slip surfaces. To simulate their irreversible and multi-step formation process, (1) the elasto-plastic constitutive model for describing material nonlinearity and (2) finite deformation scheme for tracing changes in shape and state of the ground are necessary. In this presentation, we introduce the results of the formation analysis of these structures based on our analysis code ***GEOASIA*** [1] that can consider (1), (2), the presence of pore water, and dynamics.

First, an single-phase elasto-plastic deformation analysis was performed using three plane-strain finite element meshes with different boundary conditions. SYS Cam-clay model was incorporated as an elasto-plastic constitutive model of soil skeleton. The parameters for overconsolidation exhibiting remarkable softening after the peak strength were set. The shear strain distributions indicate that the analysis without fixation of the bottom displacement exhibited pop-up, whereas the analysis with the prescription of the linear bottom displacement distribution obtained imbrication. Furthermore, the separation of the imbrication and the thrust sequence, i.e., piggyback and overstep, were affected by the presence of the end friction. We successfully simulated characteristic structures with the irreversible and multi-step strain localization in the compressed ground based on the elasto-plastic finite deformation analysis and confirmed the effect of boundary condition.

Next, the soil-water coupled analysis for the saturated semi-consolidated ground was conducted. The final shear strain distribution exhibited the formation of horizontal décollements and the accretion of the lower region to the upper region. The occurrence of the positive excess pore water pressure and the generation of a seismic wave due to brittle deformation were also solved.

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Simulation the landslide induced tsunami using integrated numerical modelling

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Key Words: *tsunami, coastal landslide, simulation, centrifuge*

Landslide events are often secondary phenomena that are triggered by other disasters such as meteorological disasters, earthquakes, and volcanic eruptions. Earthquakes can cause landslides in both onshore and offshore areas. Submarine landslides can cause tsunamis which have a catastrophic impact on coastal areas. Studying submarine mass movements and their consequences have been started in 1952 with the work of Heezen and Ewing on the Grand Banks slide and tsunami (Locat and Lee, 2009). As of today, many catastrophic submarine landslide events that generate tsunami have been reported including the dramatic landslide-generated Papua New Guinea tsunami in 1998, which devastated three villages with the loss of over 2200 lives (Tappin et al. 2008), 2018 Sulawesi earthquake with a magnitude of Mw 7.5 and tsunami hit property and life with more than 2000 fatalities. 30% of the World's population of lives within 60 km of the coast, and the understanding and hazard assessment of tsunamigenic landslides becomes very important (Yasuhiro et al., 20012).
The research applies the integrated numerical model including landslide and tsunami for simulating the complicated process of earthquake induced landslide causing tsunami. The centrifuge results will be used to validate the landslide generation tsunami model.

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Avalanching of variously shaped DEM particles in a rotating drum

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Key Words: DEM, avalanche, rotating drum, shape effects, non-convex particles

In the majority of particle simulation methods, round particles still dominate, while in actual granular materials, the particles are angular or even non-convex. Attempts to enforce "realistic behavior" with unrealistically high coefficients of rolling friction (e.g. [1]) do not necessarily result in a realistic dynamics for moving particles.

In this research, we compare how assemblies of "round", irregular convex and non-convex particles behave with respect to avalanching in a two-dimensional rotating drum using a polygonal discrete-element method based on [2]. Round particles are modelled as regular convex polygons with a high number of corners, but the differences to the ideal round shape are negligible. Solid friction is implemented via the "numerically exact" Differential-Algebraic-Equation formulation [3].

All things being equal, we find that aggregates of round particles are clearly distinguishable from aggregates of non-round particles – whether convex or non-convex – in a parameter space describing the whole of the aggregate, as well as in the behavior of avalanches, due to the differences in particle mobility and strength of solid friction. On the other hand, the deviations in the behavior between aggregates of irregular convex and non-convex particles are less marked. We find differences in the angle of marginal stability, as avalanching starts at a higher slope angle for non-convex particle aggregates compared to aggregates of convex particles, but both mixtures revert to the same steady-state angle after an avalanche. We see further differences between convex and non-convex particles in the distribution of the phasespace trajectories of the bulk center-of-mass, where the translational and the rotational energy as functions of the center-of-mass height form more compact cycles for convex than for non-convex particles, while for round particles the cycles are compact with little dependence on the drum rotation.

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Generalized FEM-DEM coupling for multi-scale modeling of granular materials using coarse-graining

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Key Words: Multi-scale modeling, Surface coupling, Volume coupling, granular media, Coarse-graining

Surface and volume coupling methods are reformulated for concurrent multi-scale modeling of granular materials. Based on a micro-macro transition technique called "coarse-graining" [1], we derive homogenization operators in more generalized forms than those reported in the literature. For surface coupling [2], coarse graining allows distributing the coupling forces beyond the finite elements that the particles are locally coupled with, namely, from contact points to their neighboring integration points. For volume coupling [3], coarse-graining is applied to enrich the homogenization/localization operations on particle-scale quantities, thereby offering a non-local coupling approach. The generalized coupling terms contain one user-defined parameter, namely, the coarse-graining width, setting a length scale for the "coarse-grained" fields. The benefits of coarse-graining in surface and volume coupling are exemplified by modeling particle-cantilever interaction and wave propagation between discrete particles and continuum bodies. We show that the CG-enriched new formulation removes high-frequency/short-wavelength numerical oscillations and gives more physical predictions in the example of particle-cantilever interaction, compared with the conventional formulation using finite element basis functions. In the wave propagation example, the numerical dissipation, which is a known artifact of the volume coupling method, is reduced with an optimal coarse-graining width. In particular, the benefit of coarse-graining appears to be significant when the waveforms become increasingly complex and contain high frequency contents.

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Ground behavior in belled pile uplifting by Discrete Element Method

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Key Words: *DEM, Aluminium Bar, Belled Pile, Pull-out Resistance*

The upward external forces applied on a pile head due to earthquakes, wind loads, etc. cause large piles pulled up in the base graound. Considering the frequency of natural disasters in recent years, it is quite important to understand the ground behavior in pile uplifting, and it is also importran to investigate numerical methods that is applicable to simulation involving ground large deformations.

In this study, the authros performed the model experiments of uplifting belled pile, forcusing on the large deformation behavior. In the experiments, both the ground behavior in belled pile uplifting and the mechanism of exerting the pull-out resistance were investigated. To understand the ground behavior further, Discrete Element Method (DEM) is adopted for the numerical analysis method, because it is expected to trace the ground behavior involving large deformations. DEM is applied to uplifting belled pile simulation, compared to the experimental results.

Model experiments of uplifting belled pile were performed with a model pile set in the circular aluminium bar laminated ground. The pull-out load and the pile head displacement were measured. Also, the spatial displacement and strain of the ground were obtained by image analysis using Particle Image Velocimetry (PIV).

2D DEM simulation was performed to investigate the stress propagation inside the ground and how the ground resists the pull-out force, because it is difficult to know the stress propagation in the experiment. The pull-out load, particle displacement and strain were simulated and compared with the experiments, resulting in that the numerical results and the deformed regions give good agreement to those of the experiments. The mean normal stress of particles and the contact force network were visualized for further consideration, and it enabled us to observe how the pull-out resistance of the ground was exerted from the viewpoint of stress propagation.

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Kinematics of Granular Materials Considering Realistic and Pseudo-Realistic Particle Morphology

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Key Words: *Discrete Element Method, Non-Convex Polygons, Node-to-Segment contact, Hopper flow*

Granular materials are a collection of discrete solids exhibiting complex behavioral responses under different physical and boundary conditions. Particle morphology is a critical component that needs to be incorporated in discrete simulations to model the micro mechanics accurately. Although there have been extensive numerical studies [1] understanding the effect of particle morphology on the overall material behavior, the complex shapes are generally modeled using multi-sphere/disc clumping methods (pseudo-realistic shapes). The primary objective of this study is to investigate whether pseudo-realistic particle morphology is capable of mimicking the kinematics of exact shapes accurately. Thus, 2D DEM simulations of conical hopper flow are carried out using realistic and pseudo-realistic particles.

Scanning Electron Microscopy images of natural sand are obtained, and particles are segmented using the modified Watershed technique, and the exact boundary pixels of each particle are extracted. The electronic noise is eliminated by smoothing spline regression combined with the cross-validation technique. For contact modeling of these non-convex irregular polygons, the node-to-segment method is employed in which the noise-free grain contours are represented locally by smoothing spline [2]. The Pseudo-realistic shapes are formed by filling the smooth outlines of grains with multiple discs. Conical hopper simulations incorporating both shapes are conducted. Linear elastic contact law is adopted with identical numerical parameters and initial void ratios. During the gravity deposition, the velocity fluctuations (linear & rotational), coordination number evolution are monitored. The velocity magnitudes towards the hopper opening are higher in the pseudo-realistic particles. The arching patterns are significantly different for both cases. Under deposition, the realistic morphologies show higher interlocking between particles. Even though the particle shape descriptors such as sphericity for both cases are same, the behavior shows considerable variations ($>$10%). Thus, it indicates that modeling a clumped system is not ideal for mimicking realistic behavior. Further, the changes in the velocity fields, coordination number, force networks (spatial & temporal) are studied as a function of roundness and sphericity of grains.

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Numerical simulation of Pile Penetration into Granular Materials Using the Discrete Element Method

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Key Words: *aluminum bar, discrete-element-method , pile-penetration*

The pile-ground interaction is one of the engineering interests that involves the ground movement. Driving precast pile and steel pipe pile drive the soil material away without boring any holes when they are installed in the ground. The ground movement in pile installations induces the increase of ground density and stress. The advantages and disadvantages of the ground change in pile penetration are discussed quantitatively but qualitatively so far. When the numerical methods are applied to pile penetration into granular materials such as soil, it is quite difficult for the methods based on the continua theory because the subdivided elements go under intensive large deformation that induces the mesh-tangling. Therefore, Discrete Element Method (DEM) is one of the engineers options used for pile penetration simulation. In this study, in order to understand the ground behavior in pile penetration, DEM is applied , and the numerical simulations are compared with experimental results of vertical penetration of piles into aluminum bar laminated ground. In the experiment, a model ground was constructed using aluminum bars, simulating the granular materials, and a steel solid pile was set above the model ground. While the piles were installed on the model ground, the penetration resistances and the photographs of the model ground were obtained. The experimental results were analyzed by Particle Image Velocimetry (PIV) to obtain the ground displacement , and the maximum shear strain were calculated. In the numerical analysis, the experimental results were simulated, and the particle displacements and maximum shear strains were obtained and compared with the experimental results. The results of the numerical analysis using the discrete element method shows that the penetration resistances, displacements, and deformation regions give close agreement to the experimental results. Physical quantities that could not be obtained experimentally, such as angular velocity of the particles and mean stress, were also calculated in the simulation. The distribution region of the maximum shear strain in experiments coincided with the angular velocity distribution region of the particles. Therefore, the rotational motion of the particles is related to the formation of the shear zone.

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Comparative analysis of oneAPI and CUDA technologies for the parallel implementation of matrix-free finite element method

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Key Words: finite element method, high performance computing, computational mechanics, solid mechanics

Modern problems [1] that use finite elements require substantial computing resources. One of the most efficient solutions in terms of the SIMD approach is the use of matrix-free methods on GPU [2]. This paper discusses the usage of the Element-by-element (EbE) method [3] for some 3D Solid Mechanics problems. The main idea of the EbE method is the absence of global stiffness matrix assembly. This results in high memory efficiency. The purpose of this work is to prove the possibility of a cross-platform implementation of the Finite Element Method using parallelism on high-performance hybrid architectures [4]. This is conducted by a comparative analysis of the performance of CUDA and oneApi technologies realizations. Obtained results make it possible to perform calculations faster than many adapted computational modern systems.

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Mathematical modeling of coupled hydro-geomechanical processes with changing properties of the medium under finite strains using high-performance computing

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Key Words: *finite strains, poroplasticity, coupling, numerical modeling, spectral element method, CUDA, GPU*

The presentation outlines an approach to solving coupled non-stationary problems of modelling hydro-geomechanical processes taking into account both physical (poroelastoplasticity) and geometrical (finite strains) nonlinearities. The considered poroelastoplastic model generalizes classical Biot's model for a two-phase liquid-saturated poroelastic medium. A distinctive feature of this model is the two-way coupling between mechanical processes occurring in a porous elastoplastic matrix and a saturating viscous fluid, which makes it possible to take into account both the effect of a change in the pore pressure of a fluid on the stress-strain state of a porous matrix and vice versa – an effect of a change in the shape of the pore space (due to the accumulated elastoplastic finite strains) on the pore pressure in a fluid. and, as a consequence of Darcy's law, on the rate of fluid flow inside the porous medium taking into account dynamic variations of both porosity and permeability.

To simulate the accumulation of elastoplastic deformations, the plastic flow theory with a non-associated plasticity law is used according to the Drucker-Prager model, which takes into account volumetric plastic deformation. In addition, within the framework of the considered poroelastoplasticity model, the nonlinear dependence of the model parameters (elastic moduli, Biot's modulus, permeability, etc.) on porosity, which, in turn, depends on the volumetric deformation of the skeleton, is taken into account. Non-recoverable plastic part of porosity variation is considered also in the suggested mathematical model.

For the numerical solution of the problem Galerkin's method and the isoparametric spectral element method are used to discretize the geometric model and equations in space on curvilinear unstructured meshes of high order (orders up to the 15th were used for solving model problems). The software implementation of the developed algorithm is performed using the CUDA technology. The spectral element mesh is naturally mapped onto the GPU's Grid, and accordingly, each spectral element is mapped onto a streaming block, within which individual SEM nodes are processed by the corresponding threads. This approach makes it possible to efficiently use the capabilities of shared memory for caching data inside a spectral element, which significantly increases the throughput of the parallel version of the algorithm.

Results of a numerical solution of several model problems are presented: a problem of the development of zones of localization of elastoplastic deformation near a well drilled in a porous rock saturated with fluid, a problem of a pure shear loading under finite strains of a model with a circular stress concentrator in its centre. The change in porosity and permeability because of the accumulation of finite plastic strains is analysed.

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Modelling of Sea Ice Formation Using the Phase-field Method

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Key Words: Sea Ice Formation, Phase-field Method

Sea ice is an important component of the global climate system, which forms naturally as seawater freezes. In polar regions, the ice forms an interface between the ocean and atmosphere, consequently influencing the exchange of heat, moisture and moment between these components. As a material, sea ice is complex as it consists of solid ice, brine inclusions, solid salts, and gas bubbles. The porosity of sea ice results from the incompatibility of salt and ice crystals, leading to brine inclusions with a high salt concentration, which changes the freezing point of seawater. The variability of the porous structure of sea ice is connected with that of temperature and salinity and profoundly influences the properties of sea ice. Other formation phenomena include the precipitation of salt ions and the liquid brine motion driven by pore pressure gradients and gravity drainage. Despite the importance of sea ice, the realistic prediction of a three-dimensional sea ice growth has not yet been achieved. It is against this backdrop that this paper models the temporal evolution and spatial distribution of the pore structure, focusing on the seawater-ice phase transition and salt-ice phase separation using the phase-field method in three dimensions.

A Viscoplasticity Model for Creep-Induced Failure of Clay

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Keywords: *Viscoplasticity, Creep Failure, Clay, Bounding Surface*

Creep-induced instability in clayey slopes generally occurs at stress levels less than the peak strength, but above the critical state line. It develops as a result of the accumulation of plastic volumetric dilation with time, leading to gradual softening and reduction of the peak strength, and ultimately failure of the soil (Tavenas et al., 1978 and 1981; Lefebvre, 1981; Hunter & Khalili, 2000). In this study, a viscoplastic model is presented for the creep-induced failure of clayey soils. The constitutive model is developed within the context of the bounding surface plasticity using the critical state theory and the consistency viscoplastic framework (Wang et al., 1997). The model enables capturing the accumulation of viscoplastic strains upon loading and unloading as well as creep rupture observed in over-consolidated clay under drained condition. In the model, the size of the bounding surface is defined as a function of viscoplastic volumetric strain and strain rate. Unlike the overstress models, the model proposed meets the consistency condition and allows for a smooth transition from rate-dependent viscoplasticity to rate-independent plasticity. Numerical results are presented and compared with the experimental data to demonstrate the performance of the model.

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Pore Pressure Parameters for Unsaturated Soils

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Key Words: Pore Pressure Parameters, Effective Stress, Hydraulic Hysteresis, Unsaturated Soils

In this study, an analytical framework developed based on the effective stress principle is presented for the determination of the pore pressure parameters in unsaturated soils under undrained condition. The concept of conservation of mass for the water phase and Boyle's law for the air phase are employed for the derivation of the pore air and water pressure parameters. The effect of hydraulic hysteresis on the effective stress parameter and the soil water characteristic curve is also considered in this study [1,2]. The proposed analytical solution is successfully validated against the experimental data presented by Campbell [3]. The results illustrate that with the increase in the saturation level of the soil, the pore air and pore water pressure parameters increase and approach unity. The outcomes indicate that the pore pressure parameters are significantly dependent on the compressibility of the soil skeleton. Moreover, the effects of hydraulic hysteresis and the initial hydraulic state, which are extensively overlooked in other studies on the pore pressure response of unsaturated soils, are investigated. The results reveal that hydraulic hysteresis can have a substantial effect on the pore water pressure parameter. However, the pore air pressure parameter is slightly affected by the hydraulic hysteresis since it is mostly influenced by the compressibility of the air phase. The results show that an increase in the degree of saturation of the soil leads to a reduction in the instantaneous settlement, and that the hydraulic hysteresis can have a significant impact on instantaneous settlement.

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A Convolutional Neural Network for predicting the eigenvalues of the 2D Helmholtz equation

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Key Words: Deep Learning, Approximation with Deep Neural Network, Convolutional Neural Networks, Eigenvalue, Helmholtz' Equation

Recently, there has been a surge of interest in utilizing Deep Neural Networks (DNNs) for a wide variety of tasks in the real world. In particular, Convolutional Neural Networks (CNNs) is regarded as a powerful tool for various fields such as image and voice recognition. The application of CNNs has been spread to computational mechanics (e.g. [1] and the references therein).

This study proposes a method to estimate eigenvalues from a given shape of the domain Ω in terms of (interior) eigenvalue problems for the 2D Helmholtz equation, following a previous attempt to estimate the solution of boundary value problems for the same equation [2]. We basically exploit an existing CNN, that is, VGG-19, and modify it so that multiple eigenvalues can be output at the same time. To obtain supervised data, we first generate a closed curve, which corresponds to the boundary of Ω, on a plane and then transform it into a 2D binary picture, where each data consists of N-by-N pixels. Finally, we solve the eigenvalue problem in Ω to calculate the lowest M eigenvalues. We considered 30,000 datasets in the following test.

In the case of $N = 224$ and $M = 1$, we measured the accuracy of our CNN with the mean absolute percentage error (MAPE). The error was 3.32% for 24000 training data and 8.63% for 6000 validation data. In our setting, both the errors saturated when the epoch was about 100, where an epoch size is defined as around 200. It seems that we cannot improve the accuracy even if the number of dataset becomes larger. On the other hand, increasing the number N of pixels much more could lead to a higher accuracy, but our computing resource prohibited us from increasing N.

In our talk, we will show the above-mentioned methodology and numerical result as well as the other results for different settings.

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A deep learning-based design approach for developing additive manufactured bone scaffolds to enhance bone ingrowth

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Key Words: *Scaffold, Deep learning, 3D printing, Bone growth, Bayesian optimization.*

Treating large bone defects remains a significant clinical challenge using existing bone tissue scaffolds [1,2]. The successful regeneration of functional bone tissues in large bone defects requires scaffolds capable of restoring the patient-specific biomechanical functions of the target bone tissues. While additive manufacturing (AM) techniques have shown great potential to fabrication of tissue scaffolds with tailored biomechanical properties, their true capability has not yet been fully exploited due to lack of effective patient-specific design methods [3]. This study proposes a subject-specific framework by combining 3D printing techniques with a novel deep learning-based design approach to fabricate functionally graded scaffolds based on Triply Periodic Minimal Surfaces (TPMS), aiming to fulfil the anticipated biomechanical requirements of target bone defects. The proposed deep learning-based design strategy coupled a Bayesian optimization algorithm [4] with finite element analyses to enable dynamic mechano-biological optimization of the scaffolds at a fairly low computational cost. A Lithography-based Ceramic Manufacturing (LCM) technique was then employed to fabricate the optimized scaffolds with functionally graded TPMS. In a representative example relating to bone scaffolding in a segmental defect in sheep tibia, the simulated bone formation results showed that the optimized scaffolds with functionally graded TPMS led to significantly enhanced bone formation outcome compared with scaffolds composed of uniform TPMS, thereby demonstrating the efficacy of the proposed design strategy. This study is expected to provide an effective tool for design and fabrication of tissue scaffolds for personalized treatment of bone defects.

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A machine learning model to forecast of a cable-stayed bridge deformation by using weather forecast data

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Key Words: *Strain Prediction, Cable-stayed Bridge, Temperature Data, Weather Forecast, Long-term and short-term memory (LSTM) network*

Strain is an important type of structural response used for structural performance evaluation and a key monitored parameter in Structural Health Monitoring (SHM) [1]. In SHM, various types of sensors are installed in the structure to measure essential structural loading and responses [2]. In this study, the time histories of stain at 10 various locations of 3 cross-sections of a real cable-stayed bridge with main span of 648m, Hedong Bridge in Guangzhou, China, is predicted according to the temperature data from local weather forecast based on the long-term and short-term memory (LSTM) network.

The strain prediction from forecasted temperature is realized by two-nested networks. Firstly, the temperature at the location of each strain sensor is predicted from temperature of weather forecast, in which the dataset of forecasted temperature and measured bridge temperature is used to train the LSTM network for temperature prediction. Then, the stain at the location of each strain sensor is predicted by the predicted temperature, in which the dataset of measured strain data and predicted temperature is used to train the other LSTM network for strain prediction.

The characteristics and correlations of forecasted and measured temperatures, or measured temperature and strain, are analysed carefully before strain prediction. It is found that the time histories of measured temperatures are generally close to forecast temperature, and the temperatures measured at different locations have similar time variations, though they may have different amplitudes. This conclusion is also basically applicable for strain. Moreover, according to the coefficients of distance correlation, the time histories of measured temperature and strain do not always have strong correlations at different sensor locations, which directly influences the prediction accuracy of strain.

According to the results of two-nested LSTM procedure, about 50% predicted bridge temperatures deviate from their measured values below 0.5℃, with about 80% under 1℃. The predicted and measured strains have consistent time variation, and the relative error is within 5% at most moments. Consequently, the proposed method successfully predicts the strains at various locations of a real cable-stayed bridge for car traffic from forecasted weather data. In the further study, the presented method will be used to predict other types of responses in the bridge, such as displacements and accelerations, based on the weather forecast information.

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A machine learning-based probabilistic computational framework for uncertainty quantification of actuation of clustered tensegrity structures

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Abstract

Clustered tensegrity structures integrated with continuous cables are lightweight, foldable, and deployable. Thus, they can be used as flexible manipulators or soft robots. The actuation process of such soft structure has high probabilistic sensitivity. It is essential to quantify the uncertainty of actuated responses of the tensegrity structures and to modulate their deformation accurately. In this work, we propose a comprehensive data-driven computational framework to study the uncertainty quantification (UQ) and probability propagation in clustered tensegrity structures, and we have developed a surrogate optimization model to control of the flexible structure deformation. An example of clustered tensegrity beam subjected to a clustered actuation is presented to demonstrate the validity of the approach and its potential application. The three main novelties of the data-driven framework are: (1) the proposed model is able to avoid the difficulty of convergence in nonlinear Finite Element Analysis (FEA), by two machine learning methods, the Gauss Process Regression (GPR) and Neutral Network (NN). (2) A fast real-time prediction on

uncertainty propagation can be achieved by the surrogate model, and (3) Optimization of the actuated deformation is carried out by using both Sequence Quadratic Programming (SQP) and Bayesian optimization methods. The results have shown that the proposed data-driven computational framework is powerful and can be extended to other UQ models or alternative optimization objectives.

Keywords: Clustered tensegrity structure, Machine learning, Uncertainty quantification and propagation, Surrogate model, Optimization inverse problem

An ANN-based model-order-reduction method for large-scale simulation and design

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Key Words: *Model order reduction, ANN, Surrogate Model, Large-scale problem, Transferability, Topology optimization*

Large-scale simulation is often encountered in many fields of science and engineering. In many cases, problems must be solved over a range of different settings. For example, during the structure design process using the topology optimization, structure evolves at each design iteration and its function/performance must be repetitively evaluated. Tackling this type of problems using conventional methods, for instance, the Finite Element Method (FEM) would entail large computational costs. In recent years, Deep learning-based models with fast online prediction such as artificial neural network (ANN) models have been developed to overcome this issue either by acting as surrogate models for function evaluation [1,2], or directly outputting design solutions [3,4]. These methods have yet to make a major impact because of the poor transferability and scalability of current machine learning models. As a result, a large set of training data is required which is infeasible for large-scale analysis and design. In this talk, we will present some recent work on the development of an efficient ANN-based model-order-reduction method suitable for large-scale problems. In particular, we will show that by using domain decomposition and coarse-to-fine mapping ANNs, surrogate models constructed using training data of one problem can be applied to a range of problems with different domain shape and size, boundary conditions and loading conditions without any re-training. As such, the transferability of the model is greatly improved.

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Artificial Intelligence-Assisted Design: A Multi-Input Neural Network-based Hull Design Assistant

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Key Words: Deep learning neural network, Artificial Intelligence, Hull deformation, Ship hull design, Total resistance

The hull design is a complicated process since a minor local change to the hull structure may significantly change the hydrodynamic performance. In order to find the hull model with the best hydrodynamic performance under the design requirements, scholars developed Computer-Aided Design (CAD) by combining computational fluid dynamics (CFD) and geometric modeling. However, the calculation workload of the computer-aided design is considerable, and in most cases, it is only applicable in the design stage with a small design space. Meanwhile, because the computer-aided design needs to perform a performance evaluation after the new ship model is obtained, it will encounter some obstacles in practical applications.

In order to assist the ship design, we applied the deep learning neural network technique, which aims to predict the total resistance of the hull model in real-time through geometric deformation parameters. However, due to the different influences of different types of geometric deformation parameters on the hull structure, its influence on the hydrodynamic performance of the hull will also be different. When processing input parameters with different influencing capabilities, traditional machine learning methods can easily become too sensitive to input parameters with high influencing capabilities. In the hull design, different sensitivity must be avoided to ensure that the designer can obtain the optimal hull according to the changing trend of the hydrodynamic and geometric modification parameters of the hull.

In this work, we simplified the geometry modification process by using two types of geometry modification parameters. The final MINN model was constructed, tuned, and trained based on the virtual reality dataset we created. The final forecast accuracy verification and sensitivity similarity verification show that the architecture of the MINN model can predict the total resistance of a hull model in real-time while maintaining the consistency of accuracy when facing different types of geometric deformation parameters. Moreover, we also proposed an example of MINN model-assisted hull design to approve the effectiveness of artificial intelligence-assisted design (AIAD). We believe our work can provide a fast and reliable assistance solution for the hull design and promote the development of AIAD in ship engineering.

Artificial neural network methods based on boundary integral equations

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Key Words: *Artificial neural network, boundary integral equation, Laplace equation*

In Anitescu et al. (2019) [1], the artificial neural network method to solve boundary value problems (BVP) for partial differential equations (PDEs) of the second order was proposed. The method is based on approximating the solution with a deep neural network and minimizing the combined error in the PDE at a set of collocation points inside the domain and the error in the boundary conditions. Such an approach presents an alternative to commonly used finite element methods. In many practical applications, BVPs can be transferred to a boundary integral equation (BIE), which is then solved by the boundary element method (BEM). BEM has a number of attractive advantages over domain-type methods, such as reduction in the dimensionality of the problem and avoidance of domain truncation error in exterior domains.

In this work, we propose an approach to approximate the solution of the boundary integral equation with an artificial neural network. Loss function represents the error in the BIE at a set of collocation points which is minimized by the appropriate weights and biases. The approach inherits the main advantages of the boundary-type methods and allows to reduce the computational cost by using collocation points on the boundary only.

Application of the method to some benchmark problems for the Laplace equation is demonstrated. A detailed parametric study is presented to evaluate the performance of the method.

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Constructing Machine-learned Interatomic Potentials for Covalent Bonding Materials and MD Analyses of Dislocation and Surface

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Key Words: *Silicon, Silicon carbide, Machine learning, Molecular dynamics, Density functional theory, Interatomic potential, Mechanical properties, Genetic algorithm*

In recent years, machine learning (ML) methodology has come to be utilized in various fields. In computational engineering, ML is effectively used for the development of interatomic potential. Such ML potentials are usually constructed on a general functional form and a large number of parameters, and many results of DFT calculations are needed for the learning.

The SNAP, or as its advanced type qSNAP, is one of the ML potentials. In this research, we actually construct SNAP and qSNAP for silicon (Si) and 3C-silicon carbide (SiC) crystal systems and confirm their reproducibility in MD simulations by comparing with an empirical potential such as Tersoff potential. Using a genetic algorithm, optimization calculations are performed so that the errors of the lattice constants and elastic moduli are sufficiently minimized.

We found that the SNAP is capable of reproducing lattice constant and elastic moduli for 3C-SiC, and the lattice constant, elastic moduli, and melting point for Si. Besides, the experimentally observed dimer structure in the free surface of Si {100}, which has not been predicted by empirical potentials, is successfully obtained by qSNAP.

Unfortunately, at this stage, the dislocation behaviour has not yet sufficiently been reproduced in either Si or 3C-SiC crystal. For Si crystal, dislocation cores are generated successfully. But, while pure shear strain is being applied to the crystal, some wrong partial dislocations occur, and the dislocation cores lose their stable shape in sliding. In cases above, we recognize that the reproducibility in the elastic region are sufficiently good, but the behaviour in the plastic region is by no means satisfactory for further MD analyses. So that, some improvement of the SNAP and qSNAP potential is expected by adding extra data on stacking defects to the learning process.

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Designing Auxetic Metamaterials using Deep Learning

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Key Words: *Negative Poisson's Ratio; Metamaterial; Generative Adversarial Network; Additive Manufacturing; Voronoi Tessellation*

As typical mechanical metamaterials with negative Poisson's ratios, auxetic metamaterials exhibit counterintuitive auxetic behaviours that are highly dependent on their geometric arrangements. Forward design is the mainstream method for designing auxetic metamaterials and includes approaches such as bioinspired methods, mathematical control, topology optimization, and Boolean and lofting operations of simple geometries. The forward design approach follows a general process: first, a structure is created, and its mechanical properties are then investigated by finite element method (FEM) simulations or mechanical testing. The mechanical properties of the designed materials are known only after time-consuming simulations or experiments. In addition, because the properties of auxetic metamaterials are determined by the geometry and assembly of periodic unit cells, the traditional methods are highly dependent on the prior knowledge of experienced designers, resulting in a limited number of design spaces.

Recent advances in deep learning have facilitated the inverse design of new materials using various artificial neural networks. This report proposes an inverse design method for auxetic metamaterials using deep learning, in which a batch of auxetic metamaterials with a user-defined Poisson's ratio and Young's modulus can be generated by a conditional generative adversarial network without prior knowledge. The network was trained based on supervised learning using a large number of geometrical patterns generated by Voronoi tessellation. The performance of the network was demonstrated by verifying the mechanical properties of the generated patterns using finite element method simulations and uniaxial compression tests. The successful realization of user-desired properties can potentially accelerate the inverse design and development of mechanical metamaterials.

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Discovery of Cell Migration Models by Data Driven Variational System Identification and Inverse Reinforcement Learning

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Key Words: Cell Migration, Variational System Identification, Inverse Reinforcement Learning

The study of cell migration is at the heart of medicinal biology, where a cell culture is observed in the presence or absence of specific drugs. Experiments suggest that migration dynamics are closely linked to certain protein levels within cells, leading to the development of kinase-pathways models for migration. However, these models are inept in predicting the tissue-scale behavior of cells. Advances in cell imaging techniques have allowed simultaneously tracking individual cells over large length scales, providing data that is amenable to continuum scale models using Partial Differential Equations (PDEs). Cells and relevant proteins can be described as a concentration field at sufficient density. In this work, we propose an Advection-Diffusion-Reaction (ADR) system for cell density, where each component of the system represents a continuum-scale homogenization of specific cell behavior. Specifically, the cell proliferation/death is modeled using reactive mechanisms while cells' directed and random motion is captured in the advective and diffusive parts of PDE, respectively.

Individual cells, however, show a much more heterogeneous behavior in terms of their affinity for random walks, directed motion, and proliferation. Therefore, the cells can be clustered into subpopulations with similar migratory features, extending the continuum scale ADR system to a multiphase one. Building upon the available kinase-pathways models, the parameters of the multiphase ADR system are proposed to be functions of homogenized fields. The data-driven Variational System Identification (VSI) approach is opted for developing a parsimonious closed system of differential equations [1]. Treating the behavior of individual cells as a Markov Decision Process (MDP) [2] and guided by the equivalence of transition probabilities in positions of cells to the homogenized behavior of Advection-Diffusion system, an Inverse Reinforcement Learning-based approach is used to study the uncertainty in the proposed ADR system.

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Graph theory-based structural analysis on density anomaly of silica glass

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Key Words: *Machine learning, Graph theory, Silica glass*

Silica glass is an ubiquitous but essential material for a vareity of industorial applications, such as optical fibers, optical lens, and substrates in semiconductor fablication. The microstructure of silica glas is composed of the tetrahedral SiO_4 units, which build up silica network by shearing their edges or corners each other. Despite the simple morphology, silica glass exhibits abnormal behaviors. For instance, as in the case of materials composed of tetrahedral units, like water, silica density becomes a minimum at temperature higher than the melting point, then increases with an increase of temperature, that is called as density anomaly. Additionally, mechanical anomaly and fragile-to-strong transition of diffusion behavior are known as typical nonlinear behaviors of silica glass.

These silica anomalies have been studied using molecular dynamics (MD) simulations. Recently, we have devloped a couple of force-fields to reproduce the energy and force calculated by the density functional theory calculations (DFT) using Bayesian optimization [1, 2]. Even though the parameter sets of the two force-fields were optimized based on the similar DFT dataset, one exhibits density anomaly of silica glass, while the other one does not. In this work, we threfore try to identify the origin of the density anomaly by comparing the glass structures obatined via MD simulations with the two force-fields.

For this purpose, the graph-based analysis method, D-measure [3], which evaluates dissimilarity (D-value) between two graphs, was employed. To find characteristics of the amorphous structure by the D-measure metric, the silica glass network was represented by a graph composed of nodes located at all silicon atom positions. The graph nodes were considred to be connected if an oxygen atom bridges two silicon atoms nearby. Then, we analyzed two types of networks: one is the global graph repreenting entire silica glass structure with considering periodic boundary conditions, and the other one is the local graph, which represents local structure extracted with a cutoff distance. The local structures were compared with template structures obtained from a variety of silica crystal phases.

Temperature dependence of the D-value when comparing with the cooled glass structure does not relate to the density anomaly. Contrarily, coesite-like intermediate-range structures, which are more dense and disordered, were identified only in the glass models exhibiting the density anomaly. The success in identifying the origin of density anomaly of silica glass confirms that the graph-based metric combined with theoretical simulations is useful as a new structural descriptor for MI of glassy materials.

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Modified Structure of Composite Neural Network using Multi-fidelity Data with Different Input Variables

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Key Words: *Multi-fidelity surrogate, Transfer learning, Deep learning, Regression model*

Recently, multi-fidelity surrogate (MFS) modeling technology that efficiently constructs surrogate model using low-fidelity (LF) and high-fidelity (HF) data has been studied to improve the predictive capability of engineering performances. In addition, various neural network (NN) structures for MFS modeling have been presented by combining with the latest developments in deep learning research. Although the existing multi-fidelity NNs have been developed with identical sets of input variables of LF and HF data, they are often different in practical engineering systems. Therefore, this study proposes a new structure of composite NN for multi-fidelity data with different input variables. The proposed network structure incorporates an input mapping network that connects input variables of LF and HF data. Even if physical relation between those variables is unknown, the input mapping network can be trained together in the process of learning the entire network model. The overall process of the proposed method is divided into two simple steps based on the concept of transfer learning. First, LFNN is trained using LF data, and it is transferred to the specific part of the proposed network. Second, while freezing parameters of the transferred NN, the remaining parameters including parameters of the input mapping network are optimized using HF data. To verify the effectiveness of the proposed method compared to a NN model with single-fidelity data, it is applied to mathematical problems with some assumptions regarding the practical engineering issue and real-world engineering problems of various tire performances.

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Nonintrusive neural optimization of topology

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Key Words: *Topology Optimization, Artificial neural networks*

Rational design of materials with high-throughput computing and machine learning has made outstanding progress in the last two decades. Yet, machine learning remains ineffective when dealing with inverse design scenarios. We propose a simple pathway where deep learning enhances topology optimization (TO) without intrusive modifications to the physics solver (e.g. finite element analyses). We aim at finding optimum topologies for nonlinear and irreversible properties when solving non-differentiable and strongly non-convex objective functions.

Physics-informed Neural Network Enhanced Reproducing Kernel Particle Method for Modeling Grain Refinement

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Key Words: *Artificial Neural Network, Reproducing Kernel Particle method, Strain Localization, Phase Field, Grain Boundary Migration*

The microscopic behaviors of materials under large deformation often entail complicated localized phenomena, such as plastic slip, grain boundary evolution/migration, micro-shearband, and micro-damage. Modeling of such localizations requires highly refined discretization for accurate prediction, which significantly increases the computational cost. While adaptive model refinement can be employed for enhanced effectiveness, it is cumbersome for the traditional mesh-based methods to perform adaptive model refinement. In this work, neural network-enhanced reproducing kernel particle method (NN-RKPM) is proposed, where the location, orientation, and the shape of the solution transition is automatically captured by the NN approximation by the minimization of total potential energy. The standard RK approximation is then utilized to approximate the smooth part of the solution to permit a much coarser discretization than the high-resolution discretization needed to capture sharp solution transition with the conventional methods. The proposed neural network approximation is regularized by introducing a length scale related to the objective dissipation energy. The proposed NN-RKPM is first verified by solving the standard damage evolution problems. The proposed computational framework is then applied to modeling grain refinement mechanisms by coupling the proposed NN-RKPM with phase field and Cosserat crystal plasticity [1], including the migration of grain boundaries at a triple junction and sub-grain formation of a material with activated slip systems, for validating the effectiveness of the proposed methods.

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Shear Stress Analysis inside CuZr-based Metallic Glasses using Machine Learning Potential

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Key Words: *Machine learning, Molecular dynamics, Metallic glass, Stress analysis*

Metallic glass (MG) with no crystalline structure is one of the promising structural materials due to its high strength, workability, and corrosion resistance. In order to expand its applicability, the mechanism of its ductility should be unveiled. Molecular dynamics simulation is a valuable tool to investigate what kind of atomic motion causes plastic behavior in amorphous materials. However, the interatomic potentials previously proposed and frequently employed, such as EAM potential, may be insufficient to capture more realistic deformaiton behaviors [1].

This study developed a machine learning-based (ML-based) potentials [2] with a particular focus on representing shear stress vs. shear strain curve with high accuracy under shear deformaiton. We have included training sets containing isotropically expanded and compressed structures, and sheared structures, obtained from density functional theory (DFT) calculation, to built the ML-based potentials. We compared the results obtained by DFT calculation, ML-based and EAM potentials: Figs. 1 and 2 show the energy curves for isotropically expanded volume and stress-strain curves averaged over six different structures, respectively. Including data under deformation allows us to reproduce the stress-strain curve obtained by the DFT calculations (Fig.2).

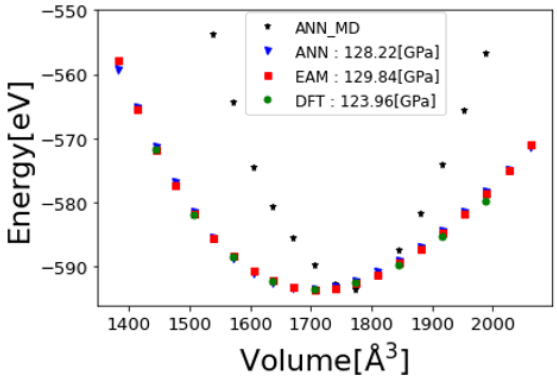

Fig. 1: Comparison of energy curve and bulk modulus for iso-expanded volume.

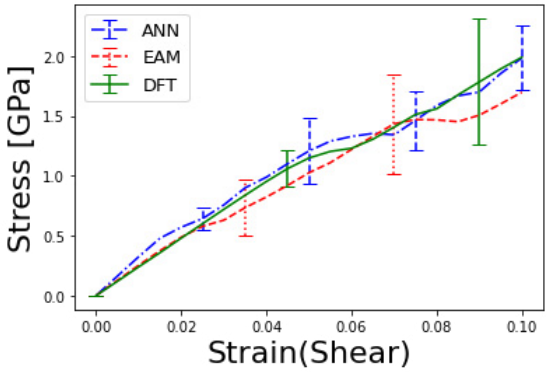

Fig. 2: Shear stress-shear strain curve for six structures.

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Combining a Long Short-Term Memory Network with 3D Simulations of Fetal and Maternal Ventricular Excitation for Fetal ECG Extraction

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Key Words: Cardiac Electrophysiology, Machine Learning, ECG, Fetal ECG

Congenital heart disease (CHD) is one of the leading causes of infant death. ECG recorded on the maternal abdomen can be used as a non-invasive diagnostics tool for CHD. However, extracting the fetal cardiac signal from the maternal abdominal ECG signal has been challenging prominently due to the low signal to noise ratio and limited access to data of the direct fetal signal which is currently measured through a scalp electrode during delivery. The goal of this study is to develop an electrophysiological model of a maternal torso with a 24-week fetus that can be used to generate realistic ECG data which will be used to train a ML network that can automatically detect fetal QRS signal.

The computational model of a pregnant torso at 24 weeks gestation is based on [1, 3, 2] and [4], which incorporates maternal and fetal biventricular cardiac geometries and additional tissue with assigned conductivities to replicate realistic electrophysiological propagation. Sinus rhythm with different rates for the maternal and fetal heart were simulated using the pseudo-bidomain formulation. Abdominal ECG recordings at locations similar to those recorded in the clinic were extracted. In this study, we measure the obtained performance metrics for fetal QRS detection from maternal ab- dominal ECG recordings using a long short-term memory (LSTM) network combined with a QRS detection algorithm trained on a combination of clinical and generated ECG recordings.

The generated maternal torso model successfully generated realistic maternal and fetal ECG signals. However, preliminary results only show an increase in fetal QRS detection accuracy to 24.62 % for a network trained on both clinical and simulated ECG recordings. To improve the accuracy, we plan to do further augmentations of the generated ECG measurements and experiment with other network architectures. However, the current results demonstrates that computer simulated ECG measurements can be used to improve machine learning models in fetal ECG extraction.

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Data Creation for Arrhythmic Risk Assessment in Post-Infarction Patients

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Key Words: *Computational cardiac electrophysiology, machine learning, data augmentation, data creation*

Background. Assessing risk for arrhythmia can be thought of, from a statistical perspective, as a classification supervised learning task[1]. However, training machine learning classifiers that perform well, whether via classical algorithms or via DLNN, requires sufficient data, the amount of which is often difficult to assess a priori and varies with the task at hand[2]. In contrast, in the health domain, clinical studies often only reflect data from relatively small numbers of patients or samples. New work into data augmentation and data creation[3] can help to increase the effective amount of data for the training of ML algorithms.

Biophysical multiscale modeling for clinical translation, now a mature stand-alone field, can offer additional insights and information about patients from first principles. These models offer mechanistic insight and, recently, also improve performance of ML and DLNN models via data augmentation and creation[4,5]. Anatomically realistic and biophysically detailed multiscale computer models of the heart are playing a significant role in advancing our understanding of integrated cardiac function in health and disease. Retrospective and prospective studies, including our own work, have previously demonstrated that computational simulations using personalized virtual heart models can be used to predict arrhythmic risk e.g., in patients with ischemic scar tissue[6] with greater accuracy than current clinical metrics.

Remodeling due to myocardial infarction (MI) significantly increases patient arrhythmic risk. Simulations using patient-specific models have shown promise in predicting personalised risk for arrhythmia. However, these are computationally- and time- intensive, hindering translation to clinical practice. Classical machine learning (ML) algorithms (such as K-nearest neighbors, Gaussian support vector machines, and decision trees) as well as neural network techniques, shown to increase prediction accuracy, can be used to predict occurrence of arrhythmia as predicted by simulations based solely on infarct and ventricular geometry.

Objective. We and others have earlier presented[5] an initial, combined image-based patient-specific *in silico* and machine learning methodology to assess risk for dangerous arrhythmia in post-infarct patients and demonstrated that simulation-supported data augmentation improves prediction models, combining patient data, computational simulation, and advanced statistical modeling, improving overall accuracy for arrhythmia risk assessment. Here, we aim to extend that work to demonstrate that advanced statistical and shape modeling techniques can critically augment sparse clinical data cohorts to improve risk assessment for dangerous arrhythmias in post-infarction patients.

Methods. MRI-based computational models were constructed from 30 patients 5 days post-MI (the "baseline" population). To assess the utility biophysical model-supported data augmentation for improving arrhythmia prediction, we augmented the virtual baseline patient population. Newly employing shape modeling techniques, patient ventricular and scar geometry in the baseline population was used to create a subfamily of geometric models, resulting in an expanded set of patient models (the "augmented" population). Arrhythmia induction was attempted via programmed stimulation at 17 sites for each virtual patient corresponding to AHA LV segments and simulation outcome, ``arrhythmia" or ``no-arrhythmia", were used as ground truth for subsequent statistical prediction (machine learning, ML) models. For each patient geometric model, we measured and used choice data features, including the myocardial volume and scar volume, as well as the segment-specific myocardial volume and scar percentage, as input to ML algorithms. For classical ML techniques (ML), we trained k-nearest neighbors, support vector machine, logistic regression, xgboost, and decision tree models to predict the simulation outcome from these geometric features alone. To explore neural network ML techniques, we trained both a three - and a four-hidden layer multilayer perceptron feed forward neural networks (NN), again predicting simulation outcomes from these geometric features alone. ML and NN models were trained on 70% of randomly selected segments and the remaining 30% was used for validation for both baseline and augmented populations.

Results and Conclusion. Stimulation in the baseline population (30 patient models) resulted in reentry in 21.4% of sites tested; in the augmented population (129 total patient models) reentry occurred in 12.9% of sites tested. ML and NN models ranged in mean accuracy from ~0.83-0.86 for the baseline population, improving to ~0.91-0.96 in all cases. We conclude that advanced statistical and shape modeling techniques can critically augment sparse clinical data cohorts to improve ML-driven risk assessment of dangerous arrhythmias in post-infarction patients.

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Efficient AI-Surrogates for Clinical Translation: Parameter Estimation and Biomechanics Assessment of the Heart

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Key Words: *Deep learning, Surrogate model, Cardiac modelling*

Great strides have been made in the understanding of the mechanical modelling of the heart over the last decades, generating a new dimension of potential tools to aid cardiologists in diagnosing heart disease. However, computational cost, infrastructure and time required by the more accurate models impede the translation of many applications to the clinic.

To tackle these limitations, we have developed AI-surrogate models, which combine dimensionality reduction, model simplification, parallel processing and deep learning techniques. AI-surrogates learn to mimic outputs of computationally intensive simulations using a simplified structure, reducing the computational demand while maintaining prediction accuracy. Additionally, AI-surrogates present the opportunity of calibrating patient-specific models and estimating tissue properties with unprecedented performance [1].

To test this approach, we created an AI-surrogate of the cardiac left ventricle (LV) to simulate its deformation through the passive filling stage of the heart cycle [2]. The AI-surrogate reproduced the ventricular displacements with an absolute error of 0.05 +/- 0.04 mm compared to the finite element method (FEM) counterpart, while reducing the computational time 10-fold. Our experiments showed that the AI-surrogate is able to characterise: the mechanical properties of the LV wall in less than 6.6 seconds; or the intraventricular pressure in less than 1.3 seconds. In comparison, a single LV deformation prediction using traditional techniques may require minutes to hours of computational time, and parameter estimation may require hundreds of such simulations. Our AI-surrogate approach could be applied to help with distinguishing specific mechanisms of dysfunction for early diagnosis of heart failure [3]. Translation to clinical practice would enable near real-time diagnosis of heart disease and potentially improve outcomes for patients.

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Model order reduction, sensitivity analysis and uncertainty quantification in cardiac electromechanics

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Key Words: Cardiac Electromechanics, Machine Learning, Reduced Order Modeling, Global Sensitivity Analysis, Bayesian Parameter Estimation

Numerical simulations of cardiac electromechanics play a crucial role in computational cardiology and precision medicine. Therefore, it is of paramount importance to develop reduced-order models (ROMs) that enable real-time numerical simulations of the cardiac function. With this aim, we propose a non-intrusive method, based on Artificial Neural Networks (ANNs), to build ROMs of cardiac electromechanics that surrogate biophysically detailed and anatomically accurate full-order models (FOMs).
The ANN-based ROM is trained from a collection of pressure-volume transients obtained through the FOM while accounting for the dependence on a set of parameters. Once trained, this surrogate model can be coupled with virtually any hemodynamic model for the blood circulation external to the heart, in the same manner as the original electromechanical model, but at a dramatically lower computational cost. Our results show that the ANN-based ROM is accurate with respect to the FOM, while requiring very small training datasets.
We demonstrate the effectiveness of our Machine Learning method in two relevant contexts for cardiac modeling. First, we employ the ANN-based ROM to perform a global sensitivity analysis on both the electromechanical and hemodynamic models. Second, we perform Bayesian parameter estimation starting from noisy measurements of relevant quantities of interest. In both these cases, by replacing the FOM of cardiac electromechanics with the ANN-based ROM, we perform in a few hours of computational time the numerical simulations that would be unaffordable if carried out with the FOM, because of their overwhelming computational cost. As a matter of fact, our ANN-based ROM is able to speedup the numerical simulations by more than three orders of magnitude.

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Multi-Fidelity Simulations of Cardiac Electrophysiology with Applications to Atrial Fibrillation

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Key Words: Cardiac Electrophysiology, Multi-fidelity, Atrial Fibrillation, Eikonal Model

Accurate simulations of the cardiac electrophysiological activity are computationally demanding due to the complexity of the equations involved. Multi-fidelity approaches can be used to reduce the computational cost. The idea is to speed up the computations by combining accurate high-fidelity models and fast low-fidelity models. These low-fidelity models are less accurate, but they are typically constructed from the high-fidelity model, therefore sufficient correlation in the quantity of interest can be expected. One clinically relevant application of the multi-fidelity approaches is atrial fibrillation. During episodes of this arrhythmia, the electrical activity of the atria is chaotic and characterized by re-entrant wavelets that self-propagate in the tissue. An appropriate high-fidelity model for this application is based on the solution of the monodomain equation for the propagation of the electric potential on the atrial surface. The eikonal equation is an approximation of the monodomain equation, based on simplified physics, that allows a fast computation of the activation times. Therefore the eikonal model can be employed as a low-fidelity model. Alternatively, one could also employ the multi-level approach, in which the low-fidelity model is based on a coarser discretization. In this work, we adapt the eikonal model to account for the re-excitability of the tissue, in order to allow the fast simulation of re-entries with this simplified model. Then, we employ the adapted eikonal model in multi-fidelity approaches for the simulation of atrial fibrillation. The multi-fidelity approaches with the eikonal model could also be applied to uncertainty quantification.

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Physics-aware Deep Learning Models for the Inverse Problem of Electrocardiography

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Key Words: Cardiac electrophysiology, deep learning, dimensionality reduction, physics-informed learning

The reconstruction of the epicardial potential field from measurements of body surface potentials is a challenging inverse problem. Classical data-driven deep learning (DL) approaches are hardly applicable in this context because they require large datasets based on invasive catheter measurements.

We present a novel DL approach based on physics-based mathematical models, balancing the lack of data with parameterized numerical simulations. Specifically, we develop auto-encoder neural networks whose architecture exploits dimensionality reduction techniques to project the epicardial potential onto a reduced subspace and approximates the forward model with a tensorial reduced basis solver. Finally, we provide the network with body surface potentials organized as time series or low-frequency discrete Fourier transform coefficients.

Numerical results on synthetic data show that the physics-aware auto-encoder neural networks are accurate and efficient tools for reconstructing the epicardiac potential from body surface potentials measurements. This approach mitigates the problem of data availability and also enables the use of low-complexity architectures characterized by a limited amount of hyper-parameters.

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Physics-informed neural network-based estimation of material properties in cardiac biomechanical models

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Key Words: Cardiac Modelling, Neural networks, Physics Informed Neural Networks, Inverse Problems

Alongside new developments in the field of biomedical imaging, computational biophysical modeling is raising a growing interest in the research community, due to the great predictive potential of physics-based mathematical models and their ability to have access to crucial clinical biomarkers non-invasively [1]. In the context of cardiovascular modelling, high-resolution and accurate multi-physics mathematical models are computationally demanding and their personalisation entails fine tuning of a large number of parameters, thus potentially limiting the translation of such models to clinical context. In this talk a novel methodology is proposed, based on emerging machine learning techniques, for the efficient and robust reconstruction of displacement fields and the local estimation of heterogeneous passive mechanical properties in cardiac biomechanical models. In more detail, physics-informed neural networks methodologies [2] are extended, adapted and combined with biophysically detailed three-dimensional cardiac biomechanical models, to generate robust and effective surrogate reduced-order models that are able to uniquely identify patient-specific physical properties. The proposed learning algorithm encodes information both from displacement data, that can be routinely acquired in the clinical setting, and from the physics of the problem, represented by a mathematical model based on partial differential equations, that acts as a regularising term. The accuracy and robustness of the proposed method are demonstrated in several benchmarks. This methodology potentially paves the way for the robust and effective identification of patient-specific physical properties.

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Physics-informed neural networks for image registration: computing cardiac strain

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Key Words: *cardiac strain, machine learning, physics-informed neural networks*

Heart disease is one of the leading causes of death in the world. Disturbances in the mechanical performance of the heart can lead to many, sometimes catastrophic, conditions. Traditionally, cardiac function is assessed with simple metrics, such as the left ventricular ejection fraction. This quantity only reflects the global function of the heart, leaving out important information. For example, it is well documented that patients with ejection fraction in normal ranges can still experience what is called heart failure with preserved ejection fraction. For this reason, more sophisticated metrics that give regional information have appeared, such as cardiac strain. Here, the deformation of cardiac tissue is characterized locally, resulting in much richer information. However, determining cardiac strain from medical images is a challenging and open problem. In this work, we focus on the computation of cardiac strain from cine magnetic resonance images, which contain a sequence of snapshots of the heart motion. These images are ubiquitous and considered the gold standard to assess cardiac function with metrics such as ejection fraction. Nevertheless, cardiac strain cannot be derived directly from these images, as they do not contain motion information. For this reason, we use physics-informed neural networks to solve an image registration problem and estimate cardiac strain from cine magnetic resonance images. Physics-informed neural networks [1] are a promising new tool to solve inverse problems, such as this one, that will allow us to infer the displacement field that transforms images between different stages of the cardiac cycle. This method allows to include the knowledge about cardiac mechanics into the learned displacement field. Here, we enforce the near cardiac tissue incompressibility to improve the accuracy of cardiac strains. We also use a space-time continuous neural network, to reflect the different motion states of the cardiac cycle. We demonstrate the feasibility of this method in a synthetic example, and we show that our method performs favorably to other registration techniques using a cardiac strain benchmark [2]. We expect that our methodology will improve the accuracy and robustness of cardiac strain measures from cine magnetic resonance images. This will pave the way to more sophisticated diagnostic tools for a range of cardiac diseases.

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Physics-informed neural networks to learn cardiac fiber orientation from multiple electroanatomical maps

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Key Words: Cardiac Fibers, Physics-Informed Neural Networks, Cardiac Electrophysiology, Anisotropic conduction velocity, Eikonal Equation

We propose a method to estimate *in vivo* the cardiac fiber architecture of the human atria from multiple catheter recordings of the electrical activation. Cardiac fibers play a central role in the electromechanical function of the heart, yet they are difficult to determine *in vivo* and hence rarely truly patient-specific in existing cardiac models.

In this work, the fibers arrangement is obtained by solving an inverse problem through the physics-informed neural network formulation. The inverse problem amounts of identifying the conduction velocity tensor of a cardiac propagation model from a set of sparse activation maps. The use of multiple maps enables the simultaneous identification of all the components of the conduction velocity tensor, including the fiber angle.

We extensively test the method on synthetic 2-D and 3-D examples, also with realistic atrial geometry. We show that 3 maps are sufficient to accurately capture the fibers also in the presence of noise. With fewer maps, the role of regularization becomes prominent. Moreover, we show that the fitted model can robustly reproduce unseen activation maps. Finally, we apply the methodology to a publicly available atrial atlas and to clinical data obtained at our center, with very convincing results.

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Active learning and integrable deep neural networks for scale bridging materials physics: From electronic structure through statistical mechanics to phase field theories and elasticity

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Key Words: Active learning, Integrable Deep Neural Networks, Cluster Hamiltonians, Order Parameters

The free energy plays a fundamental role in theories of phase transformations and microstructure evolution. It encodes the thermodynamic coupling between mechanics and chemistry within continuum descriptions of non-equilibrium materials phenomena. In mechano- chemically interacting materials systems, consideration of compositions, order parameters and strains results in a high-dimensional free energy function. Scale bridging between the electronic structure of a solid and continuum descriptions of its non-equilibrium behavior can be realized with integrable deep neural networks (IDNN) that are trained to free energy derivative data generated by first-principles statistical mechanics simulations and then analytically integrating to recover a free energy density function. Here we combine the IDNN with an active learning workflow [1,2] for well-distributed sampling of the free energy derivative data in high-dimensional input spaces, thereby enabling true scale bridging between first-principles statistical mechanics and continuum phase field models. As a prototypical material systems we focus on applications in Ni-Al alloys and in the battery cathode material: Li_x CoO_2 . Phase field simulations using the resulting IDNN representation for the free energy density of Ni-Al demonstrate that the appropriate physics of the material have been learned. This work [3] advances the treatment of scale bridging, starting with electronic structure calculations and proceeding through statistical mechanics to continuum physics. Its coupling of Cahn-Hilliard and Allen-Cahn phase field descriptions with nonlinear elasticity through the free energy density ensures a rigorous treatment of phase transformation phenomena.

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Approximating the Operator of the Wave Equation via Deep Learning

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Key Words: Deep Neural Network, Computational Science, Wave Equation

The solution of the wave equation is required in a wide variety of fields, such as seismology, electromagnetism, and acoustics. In the last few years, a number of deep learning methods have been developed for the solution of PDE-based problems, in the hopes of producing techniques that are more flexible and faster than the traditional FEM, FD, FV approaches. Deep operator networks (DeepONet) [1] attempt to solve PDEs by learning the inverse of the differential operator for a wide class of initial data, rather than learn a single solution. However, this approach is especially expensive for problems containing high frequencies, such as those with the linear wave equation.

For the approximation of the homogeneous wave equation, we present a neural network architecture that is based on the integral representation formula of the wave equation. This architecture yields a faster learning and a better generalization error when compared to the classical DeepONet architecture. Moreover, with the proposed architecture, a trained network can be retrained for solutions with higher frequencies which results in an efficient learning strategy for high frequency functions. Numerical results in 1D and 2D will be presented to analyze frequency dependent convergence of the proposed approach.

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Conditionally Parameterized, Discretization-Aware Graph Neural Networks for Scientific Computing on Unstructured Meshes

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Key Words: Graph Neural Networks, Conditional Parametrization, Surrogate Modeling

While neural networks are extensively used in surrogate and reduced order modeling of PDE solutions, they often ignore interactions or hierarchical relations between input features, and process them as concatenated mixtures. We generalize the idea of conditional parameterization [1] (CP) – using trainable functions of input parameters to generate the weights of a neural network, and extend them in a flexible way to encode critical information in unstructured meshes. Inspired by discretized numerical methods, choices of the parameters include physical quantities and mesh topology features. The functional relation between the modeled features and the parameters is built into the network architecture. Although a direct CP modification will cause a linear increase in the number of parameters with respect to the chosen parameter, such an increase can be compensated by reducing the size of the latent vectors. The method is implemented on different networks and applied to the discovery of unmodeled physics, and the simulation of unsteady flows with chemical reactions. We demonstrate that a drop-in CP modification can bring significant improvements for various existing models on several tasks essential to the modeling of physical systems. We introduce a conditionally parameterized graph neural network (CP-GNet)[2], for the approximation of complex physics on unstructured meshes, with the ability to naturally incorporate different types of boundary conditions. The CP-GNet is shown to be more efficient than the non-CP variant with only a fraction of the training data or with a more shallow architecture. Extensive numerical tests are conducted to demonstrate state-of-the-art performances on problems of different complexities.

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EM Partition of Unity Networks with Applications in Quantum Computing

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Key Words: Deep Learning, Neural Networks, Partition of Unity, Expectation Maximization, Quantum Approximate Optimization Algorithm

Using deep learning methods to approximate continuous functions and operators is a critical problem in both machine learning theory and high-fidelity real-time engineering simulation applications. Recent discoveries in neural network approximation theory motivate novel strategies that combine deep neural networks (DNNs) with basis functions from classical approximation theory, such as polynomials. Moreover, although uncertainty quantification is required in many applications, it may not be naturally produced by the approximation scheme itself [1]. Instead, this work aims at exploring a general framework based on combining DNNs with polynomial approximation schemes that provides confidence regions in addition to point estimations.

We explore the probabilistic partition of unity networks (PPOU-Nets) model of [1, 2] in the context of regression. With the PPOU-Nets, the target function at any given location is approximated by a Gaussian mixture model, where each cluster is associated with a fixed-degree polynomial. The weights of the clusters are determined by a DNN which defines a partition of unity. The target function is approximated by the weighted average of the polynomials. We propose a novel training strategy that leverages automatic differentiation and the expectation maximization (EM) algorithm. We formulate the loss function as the negative likelihood of the Gaussian mixture model. During the training, we (i) apply minibatch gradient descent to update the DNN coefficients; (ii) update the polynomial coefficients using weighted least-squares solves; and (iii) compute the variance of each cluster according to a closed-form formula derived from the EM algorithm. The EM PPOU-Nets outperform the baseline fully-connected neural networks of comparable sizes in numerical experiments of various input dimensions. We also explore the proposed model in applications of quantum computing, where the PPOU-Nets act as surrogate models to accelerate optimization over cost landscapes associated with variational quantum circuits.

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Error–in–variables modeling for operator regression

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Key Words: operator regression, error-in-variables, machine learning, reduced order modeling

Operator regression has emerged as a potential tool for reduced order modeling and PDE model discovery. Most operator regression methods learn the mapping between independent and dependent *functional* variables assuming noise only in the dependent variables. However, experimental and numerical data is often noisy in the independent variables as well. In standard regression, failure to account for noisy independent variables can lead to biased parameter estimates. With noisy independent variables, linear models fitted via ordinary least squares will show attenuation bias, wherein the coefficient will be underestimated. In this talk, we demonstrate a variation of attenuation bias for linear operator regression on functional data with white noise in both the independent and dependent variables. We also propose error-in-variables models for two operator regression methods, MOR-Physics [1, 2] and DeepONet [3], and demonstrate computationally that these new models can reduce bias in the presence of noisy independent variables for a variety of PDE learning problems, including learning the Burgers operator, the heat equation, and the Kuramoto-Sivashinsky equation.

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Hyper-Differential Sensitivity Analysis for Operator Inference

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Harnessing the full power of physics-based models for decision making is challenging but critical in many engineering analyses. Accordingly, surrogate models with reduced computational complexity are necessary to combat the prohibitive costs of high-fidelity simulations. Operator inference has recently emerged as a data-driven paradigm to non-intrusively construct physics-based reduced-order models. In this work, we use operator inference as a cost-effective approach to encapsulate dynamical constraints in an optimization setting. However, approximation errors need to be accounted for and mitigated. To that end we leverage post-optimality sensitivities as feedback mechanism to iteratively improve the training process. We demonstrate our approach on the optimization of a thermal battery that requires the modeling of multi physics phenomena.

Learning Mesh-Based Simulations using Graph Neural Networks with Physical Symmetries

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Key Words: *Machine Learning, Graph Neural Network, Equivariance*

Machine learning is a promising technology to improve computation time, accuracy, and stability of physical simulations. However, it is still an open problem to obtain more general and reliable machine learning models because of the data-driven nature of the scheme. In particular, machine learning on mesh-structured data is inevitable to realize accurate prediction because the mesh is a common data structure used in various physical simulations such as the finite element method. For machine learning models that learn mesh-based physical simulations, we put three requirements:

1. Ability to deal with mesh-structured data as an input and an output.
2. Fulfillment of constraints coming from physical laws.
3. Lightweight model to make the computation faster.

In this study, we propose a graph neural network that can reflect physical symmetry and perform prediction efficiently. Graph neural networks can deal with arbitrary meshes without any modifications in the models. Physical symmetries, such as translation and rotation, are considered through the concept of equivariance. Furthermore, we implemented differential operators in the model, which are critical to expressing spatial relationships in physical simulations. Since most physical laws are described using differential equations, it is possible to construct an efficient machine learning model corresponding to a given governing equation, which reduces computation time. We demonstrate that the proposed model learns mesh-based physical simulations with high accuracy. Besides, it can predict simulation results faster than a conventional finite element analysis software and scale up to a mesh with 1M nodes, which is not possible using existing equivariant models. We expect our model to be key to realizing more general and reliable machine learning models for physical simulations.

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Physics-informed neural network for increasing prediction accuracy of microscale variations of single plant cell during drying

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Key Words: *Physics-informed Neural Network, Moisture Concentration, Low dimensional inputs, Food drying*

Bulk level variations of plant foods during drying are mainly governed by microscale characteristic variations [1]. Investigating such microscale variations have been challenging with physics-based models due to heterogeneity of microstructures, largely unknown property data, and limitations of numerical simulations [2]. On the other hand, the development of data-driven machine learning (ML) models for predicting microscale variations has not yet been succeeded due to the inability of having a sufficient dataset for extracting an interpretable solution.

Therefore, in this work, the Physics-Informed Neural Network (PINN) capabilities are explored to improve the prediction accuracy of moisture concentration variations of a single plant cell during drying with low dimensional input data. In particular, additional information using relevant physics conditions is provided into the feedforward neural network by altering the loss function. The performance of PINN is investigated and compared against pure data-driven ML model predictions for benchmark cases. It can be highlighted that PINN with additional physics information is significantly improved the prediction accuracy even if the training data is very low, indicating the possibilities of integrating PINN for accurately investigating microscale characteristic variations of plant foods during drying.

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Deep learning in multiscale modelling of spatially tailored materials

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Key Words: *deep learning, multiscale, composites*

Riding the wave of artificial intelligence (AI), machine learning (ML) and deep learning (DL) methods have been widely used in many domains, including materials science and engineering. Here presents a novel hierarchical multiscale modeling enhanced via deep learning, which plays an important role in this multiscale framework to pass the information from the nanoscale to the microscale and then to the macroscale.

This multiscale method provides a new approach to study the mechanics of metal-ceramic spatially tailored materials, a unique type of composites, in which the volume fractions vary in space at the macroscale. Data sets, collected from molecular dynamics simulations, are used to train artificial neural networks to predict material properties at the macroscale. Then, peridynamics and finite element methods are employed to investigate the mechanical behavior of composites at the microscale, considering microstructure uncertainties. The collected data is utilized to train machine learning regression and classification models. Those predictive models are finally implemented in the macroscale simulations to study dynamical responses of composite structures under various loading conditions.

As a difference from other reported works, microstructure uncertainties are considered in this research so that an artificial neural network is trained as the machine learning classification model to predict the failure probability at the macroscale, which depends on the volume fraction and the deformation (i.e., the strain). In addition to deep learning, extreme learning is utilized for fast learning.

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Hybrid physics informed neural networks applied to two-dimensional turbulence

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Key Words: *Neural networks, turbulence, computational fluid dynamics*

Turbulence is a phenomena which is studied extensively both experimentally and numerically. In order to resolve all the length scales of a turbulent flow, expensive computational resources are required. To do this experimentally, it also involves significant resources. Recently, there has been quite lot of methods based on machine learning and deep learning which are used to enhance the retrieval of high resolution turbulent data sets. Recent work by Raissi et al[1], on physics informed neural networks (PINN) has used neural networks to find solutions to partial differential equations.

In this work, we use a hybrid PINN model to solve for two-dimensional turbulence. The aim of the work is to capture the statistical properties of turbulence. We find that the standard PINN model does not capture the two-dimensional turbulence while a modified method which uses some data from the interior of the flow domain performs well. We call this method PINN-1. In order to capture the small scales of turbulence we introduce a modified PINN denoted as PINN-2 where we train the small scales separately. We apply these two methods, PINN-1 and PINN-2 to the problem of two-dimensional turbulence in a periodic box and compare it with Direct numerical simulations. We observe the PINN-2 model outperforms PINN-1 in retrieval of solutions as close to DNS results. The turbulent energy spectra is found to match upto eight to nine decades, with only 0.1 % of training data.

We believe that such technologies can in principle be used for storage and retrieval of high resolution and high *Re* simulations where we one requires solutions at very fine time intervals and that the traditional DNS or experiments are costly.

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Liutex-based Direct Integrated Field Inversion and Machine Learning Framework for Turbulence Modeling

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Key Words: *Turbulence Modeling, Liutex, Machine Learning, Adjoint Method*

Existing Reynolds-averaged Navier-Stokes (RANS) models suffer from substantial discrepancies for separated flows, due to the Boussinesq approximation which is regarded as the limitation for modeling turbulence in complex geometries. Recently, the advance of data-augmented model with machine learning technology has shown the potential to significantly improve the accuracy of prediction for separated flows. On the other hand, a new concept of Liutex (previously named Rortex) has proposed to present the local fluid rotation, including a systematic framework of scalar, vector, and tensor forms, which provides several advantages over the traditional vortex identification criteria.

In this paper, a direct integrated field inversion and machine learning framework is presented to correct the momentum equations with the Spalart-Allmaras (SA) model. The main idea is that the feature set is constructed from the local Liutex and shear vectors, which are obtained from the Liutex-based R-S decomposition of the velocity gradient tensor. The weights of the neural network are chosen as the design variables of the framework and the training step is directly integrated within field inversion using discrete adjoint method of the CFD solver and the automatic differentiation embedded in the machine learning library. The gradient-based optimization algorithm is used to solve the field inversion problem. The proposed approach is applied to several challenging separated flows. The results demonstrate that the proposed framework can provide much improved prediction.

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Neural network supported surrogate models for particle-laden flow

This project focuses on coupling a data-driven model in conjunction with CFD (Computational Fluid Dynamics) to predict the behavior of biomass particles in a fixed bed. This problem (particle-fluid problem) can be solved by two-way coupling CFD and XDEM. Since this methodology is often computationally expensive, two solutions are proposed. Firstly, the neural network (using TensorFlow) is used as a surrogate model to replace XDEM. Afterward, this surrogate model is coupled with the CFD method to solve the particle-fluid problem employing preCICE (Precise Code Interaction Coupling Environment). An alternative approach assumes the behavior of dense particles in the biomass bed similar to that of fluid (of unknown material parameters). The neural network is used to identify the properties of the fluid. Having the properties of the fluid, the CFD method is used solely to solve the mentioned biomass problem.

Keywords: Recurrent neural network, CFD, biomass, Particle-In-Cell method

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Neural Network-Based Surrogate Models Applied to Fluid-Structure Interaction Problems

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Key Words: Neural networks, Fluid-Structure Interaction, Co-Simulation, Computational Mechanics

Traditional computational methods face significant challenges with ever-increasing complexity in the problems of engineering interest. One set of problems that suffer from this phenomenon is those where Fluid-Structure Interaction (FSI) is present. FSI simulations are traditionally time-consuming and computationally extremely expensive. Potential alternatives rely on using a surrogate model to substitute one or more systems involved. A promising approach employs artificial neural networks as the basis for such a surrogate model combined with strong physics simulations based on finite element methods (FEM).

This approach requires the seamless integration of AI algorithms and packages into the simulation workflow. Such an example is the NeuralNetworkApplication developed in Kratos [1]. This application allows the integration of every step needed to implement and integrate the aforementioned surrogate models in the simulation workflow; namely data generation, model set-up, training, testing, and coupling. The routines related to the neural networks are executed through an interface with the API Keras [3].

Mok's [2] benchmark is chosen as the study case to test the capacity of the previous method applied to FSI problems. In a first instance, the structural model in the example is substituted by a neural network-based surrogate model trained on known data while retaining the original fluid model. Additionally, a second case where a surrogate substitutes the fluid model, keeping the structural one untouched, is evaluated. In both cases, the neural network predicts the total response of the system it substitutes. Strong and weak coupling scenarios are considered. The results present improvements in simulation time without sacrificing accuracy, especially when compared with the original benchmark. This contribution discusses the influence of the original data and network architecture in the outcome of the simulation and different considerations for generating surrogate models for FSI.

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Building Better Databases to Learn From - Interatomic Potentials for Material Science and Beyond

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Key Words: Molecular Dynamics, Machine Learning, Magnetic Materials

The promise of all machine learning (ML) methods is that model accuracy can in principle be improved indefinitely so long as new training data is provided. This keeps model predictions as interpolations within the trained space rather than relying on uncertain predictions arising from extrapolations. For machine learned interatomic potentials used in molecular dynamics, there is no way to know *a priori* all the states of the material that will be observed in a large-scale production simulation. Automated training data curation either in real-time or diversity maximizing techniques are sought after to alleviate these concerns, though assembled training sets now scale with the size of the computing resources used. However, one must be aware of the limitations regarding the ML model form with respect to the complexity of the training set. This talk will overview our efforts to generate robust training sets and the computationally scalable ML models that enable a new frontier of MD simulations. Examples will be given of quantum-accurate MD predictions for magnetic materials, high-entropy alloys, as well as ML enabled predictions of matter in extreme conditions that challenge what is traditionally tractable in MD. Additionally, this talk will overview advances made in machine learned Spectral Neighborhood Analysis Potential(SNAP) for both their physical accuracy and computational performance on leadership computing platforms.

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Efficient and decision-based exploration of the high-dimensional chemical and structural design space of high entropy alloys

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Key Words: *Materials design, High entropy alloys, pyiron*

High entropy alloys consisting of five or more principle chemical elements offer a much richer design space than conventional single principle element materials. However, the structural and thermodynamic complexity of this new generation of structural materials presents a challenge to their design since experimental trial-and-error approaches, as successfully used in the past, are often no longer feasible. Ab initio approaches provide perfect tools to new design routes but face serious challenges when having to systematically sample high-dimensional chemical and structural configuration spaces. Combining advanced sampling approaches with our python based framework pyiron allows us in a highly automated way to combine first principles calculations with big data analytics and decision making. It will be shown that this combination provides a powerful path to obtain key materials design descriptors such as local order, stacking fault energies or lattice distortions, which require thermodynamic sampling over huge local configuration spaces. The flexibility and the power of these approaches will be demonstrated for a few examples: The design of high entropy alloys with superior mechanical properties or ones using magnetic configurations as additional degrees of freedom.

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Fitting and using machine learned interatomic potentials for plasticity

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Key Words: Interatomic potentials, plasticity, dislocations, cross-slip

Studying fundamental mechanisms of deformation and failure in metals an alloys necessitates dependable and accurate interatomic potentials because technologically relevant defects are orders of magnitudes above first-principles' scales. We present a Behler-Parrinello neural network based interatomic potential [1] for pure hcp Magnesium, discuss the training and validation strategy, and apply it to prismatic slip using the nudged elastic band (NEB) method. We find that a very limited training data set focused on atomic structures related to plasticity, similar to a dataset used for fitting an interatomic potential based on the modified embedded atom method (MEAM), yields very good agreement with DFT-computed dislocation structures and fracture behavior. We are able to show very good agreement with in-situ experimental observations of prismatic cross-slip [3] regarding the geometry while seeing some notable disagreement with respect to the double-kink nucleation energy.

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Optimal Ressource Allocation in Parallel Trajectory Splicing

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Key Words: task-based programming, speculation, resource allocation, accelerated molecular dynamics

Widely considered a workhorse in materials simulation, MD has struggled to maintain strong-scalability as it only weak-scales with traditional parallelization methods. One method aimed towards improving the strong-scalability of MD is Parallel Trajectory Splicing (ParSplice); a specialized MD method designed to accelerate the dynamics of rare-event systems without compromising the accuracy of MD [1]. It works by generating a large number of independently-generated trajectory "segments" in such a way that they can later be assembled into a single statistically-correct state-to-state trajectory. Due to the impossibility of deterministically forecasting the future evolution of the trajectory (which would be required to perfectly assign the execution of segments), ParSplice relies on stochastic speculation as it assigns segments via a KMC-like model that is parameterized on-the-fly. In this talk we present a method for extracting an estimate of the likelihood that any given segment will be used as part of the simulation. Then, using these probabilities, we derive an optimization framework for dynamically allocating resources among the set of possible tasks (i.e, potential segments). We detail the improvements in performance resulting from our optimized framework as compared to more naive allocation schemes including the maximum-task-throughput and minimum-time allocations. Performance results are illustrated through the use of several models of varying complexity, lending to fully interpretable results. These models enable an understanding as to when and why other allocation schemes fail, thus further highlighting the versatility/importance of our optimized allocation method. We observe that this new strategy can improve throughput up to 20x, thus greatly improving the scalability of a traditionally scale-limited application.

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An ML-based Workflow for Seismic Imaging under Uncertainty

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Key Words: *Seismic imaging, Machine learning, Uncertainty quantification*

Seismic imaging faces challenges due to the presence of several uncertainty sources. Uncertainties exist in data measurements, source positioning, and subsurface geophysical properties. Reverse time migration (RTM) is a high-resolution depth migration approach useful in extracting information such as reservoir localization and boundaries. RTM, however, is time-consuming and data-intensive as it requires computing twice the wave equation to generate and store an imaging condition. When embedded in an uncertainty quantification algorithm (like the Monte Carlo method), RTM shows a many-fold increase in its computational complexity due to the high input-output dimensionality. This work discusses an extension of the seismic imaging workflow presented in [1]. The workflow is modified to accommodate machine-learning techniques in all stages. Within a general Bayesian framework, the workflow first stage uses physics-informed neural networks for a simplified inversion, followed in the second stage by an encoder-decoder deep learning surrogate model [2] for generating the seismic images, and, in the last stage, GANs for posterior identification of seismic horizons.

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Coupling Optimal Experimental Design and Optimal Control

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Key Words: Optimal control/design, Optimal experimental design, Bayesian OED

Optimal experimental design (OED) can allow us to accurately represent engineering systems in scenarios where data is limited or significantly reduce the cost associated with performing experiments to calibrate relevant mathematical models. Furthermore, optimal control/design (OC) is a foundational aspect of operating complex systems that meet certain targets or operational requirements. Both optimization problems are challenging to solve in their own right and are often seen as independent problems related to large-scale engineering systems. However, there exists an underlying connection between these ideas as knowledge of the system, provided by the experimental data, is what is used to develop the control or design policies. Rather than focus experimental design on the intermediate step of model calibration, our work considers a more direct approach that focuses on the control policy itself. This requires a coupling of the two optimization problems, the solution of which is an optimal control policy and experimental design that are informed by one another. We develop a framework for solving an OED problem that maximizes information regarding the control objectives at the optimal control. We illustrate our approach on systems modeled using diffusive transport equations.

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Data Imputation and Bayesian Inverse using Quantum-Inspired Hamiltonian Monte Carlo

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Key Words: Bayesian inference, quantum-inspired, Hamiltonian Monte Carlo

We propose a hybrid technique combining Bayesian inference and quantum-inspired Hamiltonian Monte Carlo (QHMC) method for data intensive inverse problems. QHMC is an efficient way to sample from a broad class of distributions. Unlike the standard Hamiltonian Monte Carlo algorithm in which a particle has a fixed mass, QHMC allows a particle to have a random mass matrix with a probability distribution. Our method uses stochastic gradient optimization in QHMC to avoid calculating the full gradient on the entire dataset when evolving the Hamiltonian system. We combine the stochastic gradient QHMC and first order Langevin dynamics to obtain samples whose distribution converges to the posterior one. In many practical problems, the number of observations is large, and it is computationally challenging to apply classical inverse modeling techniques based on conventional Bayesian inference. Hence, our approach is more efficient for these tasks as it accelerates the sampling process while maintaining the accuracy. We will demonstrate the performance of the proposed approach for data imputation problems. Moreover, we combine the proposed approach with a randomized projection method for large scale inverse problems, and we will demonstrate its performance in several scientific computing problems.

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Estimation for Time-Enhancement Curves of Regions-of-Interest from Series of X-ray Projection Data Obtained from Intra-oparation

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Key Words: Time-Enhancing Curves, Intraoperative X-ray Projection, Singular Value Decomposition, Maximum Likelyhood Estimation, Regions-of-Interest

Estimating real-time time-enhancing curves (TECs) of regions-of-interest (ROI) from intraoperative X-ray projection is a big challenge in clinical practice. Traditionally, the spacial distribution of linear attenuation coefficient of each ROI was obtained from preoperative contrast-enhanced CT and combined with intraoperative X- ray projection to estimate the TECs. However, in actual surgery, there are many cases where preoperative contrast-enhanced CT cannot be obtained or there is uncertainty in the boundary of ROI due to the patient's respiratory movements. To address the problem, we developed a method for estimating TEC of each ROI when there is uncertainty in the boundary of ROI using statistical information available in advance. In the proposed method, firstly, singular value decomposition is applied on the series of intraoperative X-ray projection data, and it is decomposed into the basis of spatial distribution and the basis of time. based on this decomposition the distribution of linear attenuation coefficient and TEC of each ROI can be simply represented by linear combinations of the basis of the spatial distribution and the basis in the time direction with small number of parameters, respectively. In this framework, maximum liklyhood estimation problem under nonlinear constraints with small number of parameters can be formed. In order to verify the effectiveness of this aproach, TECs were estimated for the numerically generated fractal blood vessel model.

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Fatigue Crack Growth Prediction under Incomplete Information using Kalman Filter

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Key Words: Fatigue Crack, Prediction ensamble Kalman Filter, Incomplete Information

Predicting the growth of fatigue cracks in structures is an important issue, and many methods for predicting the growth of fatigue cracks have been researched and developed so far. On the other hand, in actual field application, the information necessary for prediction is often incomplete. For example, information such as the shape and dimensions of the target structure, the current crack length, and the magnitude of the repeated load is often accompanied by uncertainty. In this study, we developed a method for predicting fatigue crack growth under incomplete information using an ensemble Kalman filter. First, a mathematical model of the evolution of the crack length of the prediction is described based on the Paris law, and this model is used as a system model. Since the system model contains the various information mentioned above as parameters, the information with uncertainty is treated as the state quantity to be estimated together with the crack length. Based on the above framework, the nonlinear state estimation problem is set and the estimation is performed by the ensemble Kalman filter. The effectiveness of this method was verified by performing a numerical simulation for the fatigue crack growth problem of the compact tension specimen as an example.

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Projected Variational Methods for High-dimensional Bayesian Inference

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Key Words: Bayesian inference, variational inference, transport map, curse of dimensionality, covid-19

Bayesian inference provides an optimal framework to learn models from data with quantified uncertainty. The dimension of the model parameters is often very high or infinite in many practical applications with models represented by, e.g., differential equations or deep neural networks. It is a longstanding challenge to accurately and efficiently solve high-dimensional Bayesian inference problems due to the curse of dimensionality—the computational complexity grows rapidly (often exponentially) with respect to the parameter dimension. In this talk, I will present a class of transport-based projected variational methods to tackle the curse of dimensionality. We project the high-dimensional parameters to intrinsically low-dimensional data-informed subspaces and employ transport-based variational methods to push samples drawn from the prior to a projected posterior. I will present error bounds for the projected posterior distribution measured in Kullback–Leibler divergence. Numerical experiments, including inference of covid-19, will be presented to demonstrate the properties of our methods, including improved accuracy, fast convergence with complexity independent of the parameter dimension and the number of samples, strong parallel scalability in processor cores, and weak data scalability in data dimension.

This talk covers the following joint work:

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Regularization Method using Crack Growth Candidate Solutions in Crack Identification Inverse Problem

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Key Words: Crack Identification, Numerical Simulation, Inverse Problems, Candidate Solution

The problem of identifying cracks inside a structure is an important engineering issue. Since the inverse problem of identifying cracks inside a structure is ill-conditioned, it is necessary to apply some regularization method for accurate identification. In this study, we have developed a novel regularization method using crack candidate solutions for the crack identification inverse problem. In this inverse problem, we focus on the changes in strain on the surface of the member that occur before and after the occurrence of cracks, and identify the shape and position of the crack. First, a crack growth simulation is performed to generate candidate solutions for possible cracks. By using the generated candidate solution as prior information, the solution space is limited and the problem is regularized. In order to confirm the usefulness of this method, cracks were identified from the changes in the surface strain of the tensile test piece including cracks.

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Scalable Statistical Finite Elements via Partial Differential Equation Representation of Matérn Fields

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Key Words: Statistical finite element method, Matérn kernel, fractional stochastic partial differential equations, sparse precision matrices.

The increased availability of observation data from engineering systems in operation poses the question of how to incorporate measurement data into finite element models. The recently proposed statistical finite element construction (statFEM) provides a principled means to synthesise measurement data and finite element models [1]. The uncertainties present in the data, the mathematical model and its finite element discretisation are taken into account using a Bayesian statistical framework. The posterior densities of the finite element solution, model misspecification error and the noise are inferred from the data by updating their respective priors. The corresponding likelihood function depends on the data and the finite element model. In the present work, we assume that all the random fields are Matérn fields and parameterise them using their fractional stochastic partial differential equation (SPDE) representation leading to sparse precision matrices. Consequently, all the precision matrices are sparse, and the precision matrix of the posterior can be obtained using only sparse matrix operations. In addition to improving scalability, the SPDE representation provides a reasonable description of covariance structures on non-Euclidean domains, accounts for smoothness variability in the data and naturally extends to non-stationary random fields. We demonstrate the scalability and efficacy of the proposed approach with several examples from structural mechanics.

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Using Manifold Learning to Enable Computationally Efficient Stochastic Inversion with High-dimensional Data

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Key Words: *Uncertainty Quantification, Inverse Problems, Dimension Reduction, Machine Learning*

The increased usage of computational models for applications ranging from engineering to healthcare has been paired with an increasing need to quantify the numerous uncertainties influencing the input parameters to these models. Data-consistent inversion is a measure-theoretic approach to solving stochastic inverse problems that is especially suited to quantifying aleatoric, or irreducible, uncertainties in such parameters of interest [1]. In the data-consistent approach, initial or prior beliefs about input model parameters are summarized with probability distributions and updated using observed data on output quantities of interest. However, in contrast to Bayesian methods which use the ratio of the joint data-likelihood to a constant evidence term, the data-consistent approach updates the initial probability distribution of parameters using the ratio of the distribution of observed data to a predicted distribution of data. In practice, these predicted and observed probability distributions for the quantity of interest are approximated using kernel density estimates utilizing the push-forward samples from the model and observed data, respectively. This yields a solution to the inverse problem that is consistent in the sense that the push-forward of the updated probability distribution matches the observed distribution of data.

While this approach has been successfully applied in a wide variety of contexts, it has been practically limited to problems where the dimension of the observed quantity of interest is low or reduced by choosing a few components of a principal component analysis [2]. For higher-dimensional quantities of interest, accurately estimating the observed and predicted probability densities becomes a significant challenge, especially if the amount of data is limited or if kernel density estimates, which are well-known to scale poorly with respect to increasing dimension, are utilized. In this work, we employ nonlinear dimension reduction to map the quantity of interest to a lower dimensional space, and then utilize density estimation on the reduced data space. Specifically, we show how nonlinear methods of so-called “manifold learning” are suitable for physical systems where the effective dimension of the quantity of interest is low, even though the natural dimension of the measured quantities is high [3]. By applying such dimension reduction techniques to the quantity of interest, we demonstrate that we can obtain accurate solutions to the stochastic inverse problem using the data-consistent approach in high-dimensional applications.

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Variational Bayesian optimal experimental design for the discovery of electro-deposition process models

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Key Words: *Uncertainty quantification; Bayesian inference; Optimal experimental design; Nonlinear experimental design; Stochastic approximation; Shannon information; Variational inference, Industrial Applications,*

Electro-deposition is a process widely used in the automotive industry to create a coating film on the vehicle body to protect it from corrosion. This process is particularly challenging to model and optimize due to the uncertainty associated with the physical properties of the coating film during the process and lack of understanding of the physics of the process. The deposition onset of the coating film is associated with threshold parameters leading to discontinuities in the model output, making it difficult to infer such parameters. To efficiently reduce uncertainty, we may design new experiments such that the measurement data provide the greatest value. This is quantified as the mutual information between the parameters and data under different conditions, which is also the expected information gain on the model parameters from data [1]. The overall utility function is estimated through a nested variational inference loop, allowing us to accommodate high-dimensional parameter spaces needed for capturing the effects of missing or inadequate physics [2]. We further employ surrogate models based on random forest or neural network to accelerate the overall computation. The impact of different approximations in the variational inference and surrogate model is carefully assessed.

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Deep learning framework for material design space exploration using active transfer learning and data augmentation

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Key Words: *Instructions, Multiphysics Problems, Industrial Applications, Covid-19*

Neural network-based generative models have been actively investigated as an inverse design method for finding novel materials in a vast design space. However, the applicability of conventional generative models is limited because they cannot access data outside the range of training sets. Advanced generative models that were devised to overcome the limitation also suffer from the weak predictive power on the unseen domain. In this study, we propose a deep neural network-based forward design approach that enables an efficient search for superior materials far beyond the domain of the initial training set. This approach compensates for the weak predictive power of neural networks on an unseen domain through gradual updates of the neural network with active transfer learning and data augmentation methods. We demonstrate the potential of our framework with a grid composite optimization problem that has an astronomical number of possible design configurations. Results show that our proposed framework can provide excellent designs close to the global optima, even with the addition of a very small dataset corresponding to less than 0.5% of the initial training dataset size.

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Designing staggered platelet composite structure with Gaussian process regression-based Bayesian optimization

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Key Words: *Bioinspired composite, Staggered platelet structure, Gaussian process regression, 3D printing, Bayesian optimization*

The staggered platelet composite structure, one of the most well-known examples of biomimetics, is inspired by the microstructure of nacre where stiff mineral platelets are stacked up with a small fraction of soft polymer in a brick-and-mortar style[1-2]. Significant efforts have been paid to establish a framework to design a staggered platelet pattern that achieves an excellent balance of toughness and stiffness. However, because no analytical formula for accurately predicting its toughness is available due to the complexity of the failure mechanism of realistic composites, existing studies investigated either idealized composites having simplified material properties or realistic composites designed by heuristics. In the present study, we propose a Bayesian optimization framework to design staggered platelet structure that renders high toughness. Gaussian process regression (GPR) is adopted to statistically model the complex relationship between the shape of staggered platelet array and the resultant toughness. Markov Chain Monte Carlo algorithm is used for the determination of optimal kernel hyperparameter set for the GPR. Starting off with 14 initial training data collected with uniaxial tensile tests, GPR based Bayesian optimization that uses expected improvement (EI) acquisition function is carried out. As a result, it was possible to design a staggered platelet pattern that has toughness 12% higher than the best sample in the initial training set, and this improvement is achieved after 5 iterations of our optimization cycle. As this optimization framework does not require any material theories and models, this process can be easily manipulated and applied to various other material optimization problems, based on a limited set of experiments or computational simulations.

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Generative Design of Three-Dimensional Interpenetrating Phase Composite Materials

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Key Words: *Interpenetrating Phase Composite, Generative Design, 3D architecture, Elastic Modulus*

Interpenetrating phase composites (IPC) are a type of architected materials, consisting of multiple phases with topological continuity and microstructural interconnectivity[1]. While the properties of each component in an IPC can be preserved to a large extent, the overall performance of the composite is highly tunable, which makes it advantageous in a wide range of applications[2,3]. However, due to the intrinsic structural and compositional complexity of IPCs, there is still lack of clear principles to guide the optimization of the composites based on a comprehensive description of the structure-performance relationship. In this study, high throughput finite-element-method (FEM) calculations in conjunction with generative machine learning models were adopted, for investigating the correlations among the target mechanical properties, the compositions of the components, and the patterns of material microstructures. The training dataset was constructed by a combination of high-symmetry patterned IPCs and randomly generated configurations followed by topology optimization. Next, extended from the current generative design approach for 2D patterns[4], the 3D structures were transferred to multi-slice images that were then learnt by deep-neural-network based models inspired by those in medical imaging. Finally, new IPCs with promising mechanical properties were proposed, where critical local structural features were identified and analyzed. This FEM-ML framework is expected to provide useful guidelines for 3D materials design, as well as throw light on the mechanistic understandings on IPCs.

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Generative Machine Learning-Based Optimization for Composites with High Impact Performance

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Key Words: *Ballistic performance, Composite, Machine learning, Optimization*

High impact performance is one of the essential mechanical properties for designing structures such as armor that may be subjected to high velocity or ballistic loading. Understanding the fundamental mechanisms and behavior of materials when undergoing high velocity loads is critical to building next generation impact resistant materials. Previous works in the field have created composites inspired from natural materials for better impact performance under dynamic loading. However, most of the literature have focused on low-velocity loading conditions or limited design spaces have been explored due to an extremely large design space of the microstructure of composites. In this work, we aim to design novel two-phase composite microstructures with superior impact resistance when undergoing high velocity loads (>500 m/s). Our approach involves a generative machine learning-based optimization approach that incorporates a genetic algorithm and deep neural networks. Thousands of random microstructures pixelated as soft and stiff square elements are generated and their impact performance is calculated using finite element method (FEM) for training data in our machine learning model. Convolutional neural networks (CNNs) are then employed to study the complicated correlation between the high dimensional input (microstructure) and output (residual velocity and displacement). The trained CNNs predict the performance of composites much faster than FEM which requires high computational cost. Leveraging the fast inference and high prediction accuracy of CNNs, we utilize them as surrogate models combined with genetic optimization to accelerate the design process. The genetic algorithm generates new designs which have higher impact performance than that of training datasets based on greedy decisions made by CNN. The new input datasets are then fed back into the model for active learning to improve the prediction accuracy of the CNN. Results show that our final designs have remarkably improved impact performance compared to conventional composite designs and we discuss the strength of machine learning in accelerating the optimization process.

Image-based Structural Composite Design and Mechanical Characterization via Image-to-particle Conversion and GPU-accelerated Lattice Spring Fracture Simulation

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Key Words: *Composites, Mechanical Characterization, Simulation, Parallel Computing, CUDA*

To extend and expedite the design of structural composites, a fast and high-fidelity framework to predict the mechanical responses beyond elasticity becomes essential in the design cycle. One of the viable numerical approaches is lattice spring model (LSM), a coarse-grained particle spring network capable of predicting the elastic and fracture behaviors of complex composite geometries. Due to the increasing geometric complexities and configurations for material design, a large number of particles are often needed to reach convergence in LSM simulations, greatly abating the potential as an integral part of data generation pipeline for machine learning aided design. We have recently reported ImageMech—a novel platform that converts image-based geometries into particle models and simulates the mechanical responses under external loading. In our platform, the CUDA-accelerated C++ code for LSM simulation (CuLSM) outperforms the CPU-centered code by a remarkable speedup up to two orders. The platform enables a faster and more flexible mechanical characterization on structural composites and holds the key for faster exploration over the composite design space.

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Intelligent Composites Forming - Simulations For Faster, Higher Quality Manufacture

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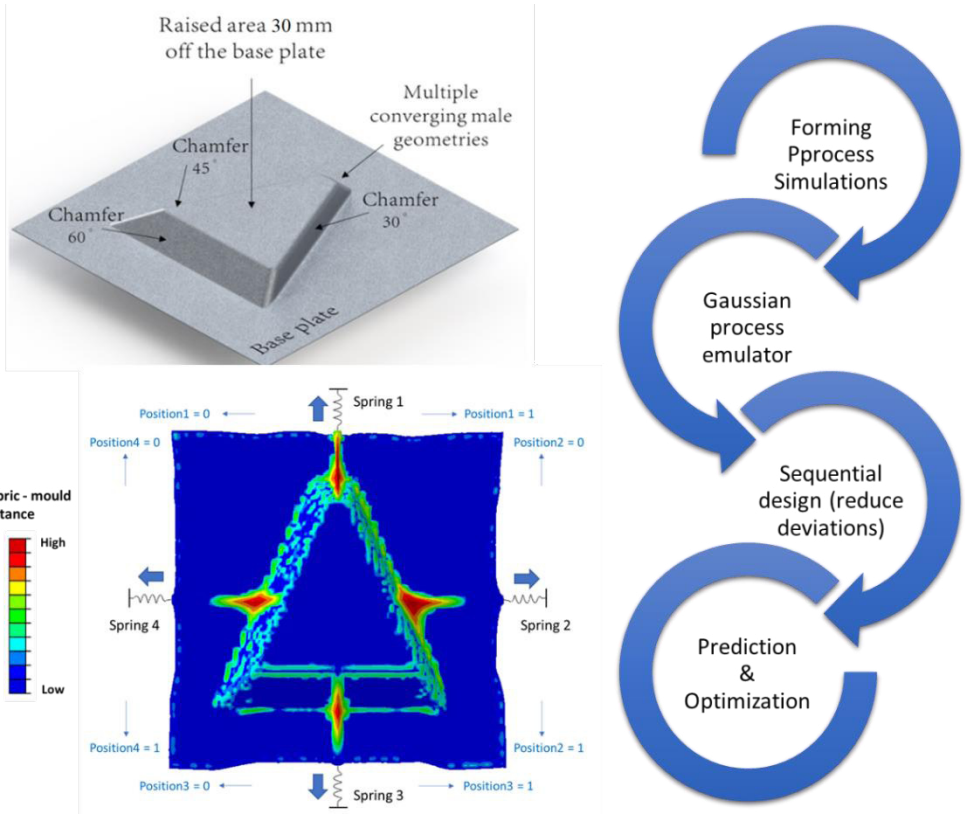
Key Words: *Composites Forming, Finite Element Analysis, Gaussian Process Emulator, Surrogate model*

In the field of composites, infusion techniques are a cheaper manufacturing alternative to autoclave moulding of prepreg. However, the latter is often the favoured manufacturing route in the aerospace sector as it allows for the production of better quality parts (in this industry passenger safety is paramount). One of the challenges with infusion techniques is the high deformability of the dry fibrous precursor material, which makes it susceptibly to defects and part variability. In particular, prior to the infusion phase, the dry fibrous reinforcement, is formed to shape; the quality of the final part is sensitive to both variabilities in materials and the forming process itself. If the material and process (including their variabilities) are not understood or controlled, this can result in design tolerances not being met, reducing composites weight saving advantages through requiring "over design".

In the last two decades, FE-based methods have been developed to help optimise process conditions for the best part quality. However, these require large number of explicit iterations because of significant dynamic and non-linear behaviour, making them very time-consuming especially for complex models. The design space and the number of process parameters that can be optimised can be quite large (e.g. bagging material, boundary conditions etc) making the optimisation process computationally intensive. Therefore, an intelligent strategy must be used to design these simulation tests and conduct optimisation with the computational cost as low as possible.

In the present contribution, FE simulations of a forming process of an industrial inspired geometry are conducted based on forming simulation tools developed at the University of Bristol [1-2] to produce a small dataset required to build an emulator for process optimisation. The simulations consider four tensioning springs attached at the boundaries of the textile material to provide tensile force during forming process (see the figure), of which the positions and stiffnesses are variables. A Gaussian process emulator (surrogate model) is then built [3-5] to model and optimise these variabilities. Gaussian emulators excel in situations where only small datasets are available. They also have the added benefit of uncertainty quantification, thus no manipulations are required for inclusion of variability. This work will present the methodology for building such emulators for optimisation of composite manufacturing simulation, including

the possibility to improve emulator performance through sequential design. The long term ambition of this work, is to build a fully autonomous forming rig with embedded sensors and active controls where the manufacturing conditions are adapted on the fly and defect formation mitigated based on rich, live experimental data feeding into real-time simulation and optimization of the process.



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The mechanism of Activated carbon to removal Nano-plastic from Molecular dynamics approach

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Key Words: *Nano-plastic, Activated carbon, Adsorption mechanism, Molecular dynamics*

In recent years, many plastic materials had been produced and widely used in our daily life. However, there is an increasing concern on the subject of plastic pollution. The fragment of plastic can be easily delivered and accumulated between animals and the environment. Nano-plastic is a fragment of plastic that assemble into small particles. The Nano-plastic particles size range between 1 nm to 1000 nm. Due to its small size, nano-plastic could penetrate into cell membranes and affect protein structures and functions in our body. Activated carbon (AC) is the powder which has high porosity and surface area to adsorb molecules and is widely used for filtration and purification. Because of its excellent property, many wastewater or gas system filters are based on AC.

In this study, we focus on the nano-plastic property in water and investigate the interactions between nano-plastic and AC by using the full atomistic approach. We construct four common types of nano-plastic: polyethylene (PE), polystyrene (PS), Nylon66, and polyethylene terephthalate (PET) with different particle sizes. Through analyzing the diffusion property of particles and their adsorption mechanism on AC, our results provide fundamental insights into the molecular mechanism of nano-plastic, which can further lead to new inspirations for resolving these environmental issues.

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Transfer learning using homogenization theory for efficiently predicting elasto-plastic response of particle/short fiber-reinforced composites

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Key Words: *Homogenization, Transfer learning, Short fiber-reinforced composite, Machine learning, Deep Neural Network, Adaptive incrementally affine*

We recently proposed the adaptive incrementally affine method as a novel homogenization scheme that enables accurate prediction of the nonlinear mechanical response of particulate-reinforced composites under cyclic or multiaxial loading conditions [1]. However, being a mean-field homogenization method that relies on the solution of Eshelby's inclusion problem, the aforementioned method does not provide an accurate prediction when the shape of the reinforcement has a high aspect ratio or the interaction among reinforcements becomes significant. Herein, we propose a combined theoretical and data-driven approach in which the homogenization method is followed by transfer learning to enhance the prediction of the nonlinear mechanical response of particle/short fiber-reinforced composites [2]. We first trained a deep neural network (DNN) with a massive stress-strain curve dataset of a composite subjected to uniaxial loading and cyclic loading in the elasto-plastic regime based on the adaptive incrementally affine homogenization method; then, we fine-tuned the pre-trained DNN via transfer learning with a relatively small dataset based on time-consuming three-dimensional (3D) finite element analyses (FEA). The transfer learning approach exhibited better predictive performance than the DNN directly trained only with the FEA dataset did, for a wide range of reinforcement volume fractions and shapes. With transfer learning, the DNN exploits the knowledge learned from the homogenization theory to perform a new learning task on a small dataset from 3D FEA. The combined theoretical and data-driven approach proposed herein can be extended to the prediction of various physical properties of composites in regimes where the applicability of the homogenization theory is limited and where direct experiments or numerical simulations require excessive time or cost to generate a large dataset.

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A Basic Study on Prediction of Airborne Chloride by Machine Learning and Numerical Simulation

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Key Words: *Chloride Attack, Airborne Chloride, MSM, Numerical Simulation, SWAN*

Reinforced concrete structures in coastal areas are susceptible to chloride attack caused by airborne chloride. Therefore, quantitative and accurate prediction of the amount of airborne chloride will enable rational construction design and maintenance management against chloride attack and extend the service life of buildings. However, a method with high prediction accuracy has not yet been established because of the complexity of environmental factors involved in airborne chloride. The authors have been predicting the airborne chloride using machine learning, based on data on airborne chloride observed in various regions of Japan and environmental data such as wind and waves available on the Internet [1][2]. As a result, the predicted values generally captured the actual measured values, but the accuracy of the prediction could not be determined accurately because the observation sites of the environmental information used and the observation sites of the airborne chloride far apart. In this study, wind data were obtained using the Japan Meteorological Agency (JMA)'s Grid Point Values (GPV) produced from the Meso Scale Model (MSM) (: MSM-GPV), which is thought to better reproduce the environment of the observation site for airborne chloride. For the wave data, we used the open-source Simulating WAves Nearshore (: SWAN) developed by Delft University of Technology in the Netherlands. For other environmental data, we used data available on the Internet as in previous studies. The training data for machine learning (airborne chloride data) used in this study are those observed at the Benoki exposure site in Kunigami Village, Okinawa Prefecture. The period covered is from January 2008 to December 2021. From these data, we predicted the airborne chloride using PyCaret, which can compare multiple machine learning programs at once. The results showed that the predicted values generally captured the trend of the measured values. In addition, the prediction accuracy of airborne chloride using MSM-GPV and SWAN was high.

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A wavelet-based three-dimensional Convolutional Neural Network for superresolution of turbulent vorticity

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Key Words: *superresolution, wavelets, isotropic turbulence, vortex structures*

We examine whether superresolution of small-scale turbulence can well preserve the position and structure of coherent vortices in three-dimensional (3D) turbulence. Convolutional Neural Networks (CNN) are used, because they can well learn characteristic spatial structure. Here we develop a wavelet-based 3D CNN (WCNN3d) for superresolution of coarse-grained data of homogenous isotropic turbulence. Wavelets are well-localized functions in scale and position and yield an efficient orthogonal multi-scale representation of the spatial structure of the vortices using the fast wavelet transform, see e.g. Ref. [1].

Recently, Kim et al.[2] applied Cycle GAN to perform superresolution of turbulent flows and showed that turbulent statistics, such as probability density function (PDF) of vorticity and energy spectra in two dimensions are well preserved. However, the positions of vortices are not well kept.

We performed direct numerical simulation (DNS) of turbulence in a periodic box at 512^3 grid points. The coarse-grained data are then obtained by applying a Gaussian low pass filter. The 512^3 data are divided into 8^3 subcubes with 64^3 grid points each. Then, we apply the discrete wavelet transform to each subcube and subsequently use 3D CNN. To this end PyWavelets,[2] an open source of Python, is used. For the wavelets we choose 'coif2' (called Coiflet 12 in Ref. [1]) having four vanishing moments and impose 'symmetric' boundary conditions in the wavelet transform of the subcube data.

We assess the performance of our WCNN3d in terms of 3D visualization of vorticity, PDF of vorticity, enstrophy spectra, etc. We find that WCNN3d well reproduces the vorticity statistics and the positions of the vortices from coarse-grained vorticity fields. Moreover, we also show that without wavelets, 3D CNN does neither well reproduce the vorticity statistics nor the vortical structures. We will discuss the influence of choice of low-pass filters on WCNN3d and the influence of the Reynolds number.

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An Examination of Floating-point Precision for Super Resolution of Micro Meteorology Simulations

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Key Words: *Convolutional, Neural network, Super resolution. Floating point, Precision*

A real time prediction of micro meteorology is expected to provide a valuable information such as temperature distribution to prevent heatstroke. However, the calculation cost of high resolution micro meteorology simulation is extensive. In recent years, the convolutional neural network (CNN) have achieved the significant improvement in graphic image. We had presented the Image-SR which predicts a high resolution temperature from a low resolution micro meteorology simulation using the super-resolution technique based on the CNN. The CNN requires more GPU memory in training of supervised machine learning as number of training data increases. To reduce the amount of GPU memory usage as well as calculation time, we examined the effect of changing floating point precision and other factors. The results indicated that the mixed floating point precision would be sufficient for the inference accuracy. In addition, the modification of hyperparameter and network architecture enables good performance especially in half precision.

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Analyses of Odor Gas Advection around the Miura Peninsula Using High-Resolution Meteorological Simulation

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Key Words: *Mesoscale Atmospheric simulation, Gas Advection, Lagrangian Particle Tracking, Environmental Flows*

Since June 2020, complaints about a strange smell of unknown origin have been repeated around the Miura Peninsula in Kanagawa Prefecture, which is located to the south of Tokyo. According to the Kanagawa Prefectural government, 22 cases of odor reports occurred during the period from June 2020 to October 2022 [1]. However, the clear source of the odor gas has not been identified yet. Therefore, in order to contribute to the elucidation of the source of odor gas, a high-resolution meteorological simulation is performed using the Multi-Scale Simulator for the Geoenvironment (MSSG) [2, 3, 4] for the first case on June 4, 2020. In this case, the number of odor reports to the fire department exceeded 200, and the reporting areas spread more than 15 km from north to south in the cities of Miura and Yokosuka.

The MSSG is a multiscale atmosphere-ocean coupled model, which can cover the global, meso-, and urban-street scales. Here, a mesoscale atmospheric simulation is performed for the largest domain of 350 km × 422 km with 3 nested domains. The horizontal grid spacing of the innermost domain is 100 m. To analyse the advection of odor gas near the ground surface, the Lagrangian particle tracking method is used. Particles are transported by winds on complex terrain and turbulent random perturbation.

To investigate the reason of widespread odor report locations, particle tracking is conducted backward in time from odor report locations. The results suggest that the odor gas is transported from the south edge or further south of the peninsula. Particle tracking is then conducted forward in time from the southern sea of the peninsula. Temporal change of the obtained particle distribution near the ground surface qualitatively agrees with the actual temporal change of the odor report locations. These results indicates that the odor gas could have been transported from the south edge or further south of the Miura peninsula by weak winds near the ground surface.

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Direct numerical simulation of turbulent mixing in a heated swirling jet issued into a cross-flow

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Key Words: *Turbulent mixing, Swirl jet, Direct numerical simulation*

A jet issued into a cross-flow, or also called a transverse jet, is a common phenomenon in engineering applications [1]. The transition from a laminar to turbulent jet often occurs and the intricate turbulent motions enhance the mixing of fluid, which also contributes to the transfer of heat, momentum, and energy. The turbulence generated in the transverse jet plays important roles in, for example, the diffusion of chimney plumes and the flow induced by air-cooled heat exchangers used in various types of plants, where the jet flow issued into the atmosphere often has a swirling motion generated by an axial fan. Therefore, swirling jets issued into a cross-flow are important in the industrial application of micro-meteorology prediction.

The present study performs direct numerical simulations (DNSs) of a swirling jet in a cross-flow and a conventional transverse jet without swirling motion, where the jet fluid is slightly heated. Here, the temperature difference between the jet and cross-flow is assumed to be small enough to treat temperature as a passive scalar. The DNS code solves the incompressible Navier-Stokes equations and the transport equation for temperature with the fractional step method, where the second-order central difference and the 3rd-order Runge-Kutta method are used for spatial and temporal discretizations, respectively. The same code has been used in our previous studies [2,3]. The DNS data is analyzed to investigate the turbulent mixing in the swirl jet, where the effects of swirling motion are evaluated by comparing the results with a conventional transverse jet. Flow visualization shows that the swirling motion significantly suppresses the vertical heat transport by the turbulent jet and the high-temperature fluid from the swirling jet tends to stay near the ground. The effects of the swirling motion are further investigated by the statistics related to turbulent mixing.

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Drag Coefficient of Fractal Trees: Investigation into Geometric Invariability

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Key Words: trees, multi-scale, adaptive-mesh, CFD, drag, fractal, l-system, micro-meteorology

Modeling the aerodynamic behavior of trees has remained challenging in great part due to their multiplicity of scales owing to self-similar fractal structure and dynamic response to wind [1]. We investigate the drag coefficient for different complexities of fractal trees in order to produce models of standalone trees found in urban environments. The computational fluid dynamics code WABBIT [2], developed for the study of insect flight [3] is utilized for its ability to resolve multiple scales with an adaptive grid. Various tree like geometries are modeled using an iterative algorithm capable of generating fractal structures [4]. Drag is found to reduce linearly as tree complexity increases, despite a non-linear increase in frontal area. We propose that trees have naturally selected for a fractal arrangement in dense canopies to slow inter-canopy flow and reduce wind loads. The outlook is to find if a geometrically independent quantity, as the fractal dimension, that can be used to model aerodynamically similar trees in urban micro-meteorological simulations.

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Highly Resolved Regional Climate Simulations over Southern Kanto in Japan with Pseudo Global Warming Method

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Key Words: *Pseudo Global Warming Method, Dynamical Downscaling, Mesoscale Atmospheric Simulation, Adaptation Measure*

Mitigation measures for climate change are globally discussed so far, and today adaptation measures are also important issues for local governments. Recently the planning of the adaptation measures gets to be supported in information platforms (e.g. A-PLAT [1]) by national institutes. However, the climate information is not enough for planning adaptation measures because the spatial resolution of the climate information is coarser than municipal area size. Thus, highly resolved climate information is required. Here we have performed regional climate simulations using the Multi-Scale Simulator for the Geoenvironment (MSSG) [2] on Earth Simulator 4. Dynamical downscaling from GPV data of Japan Meteorological Agency has been conducted. The horizontal spatial resolution is 320 meters. We have also considered the climates both 2 K and 4 K warmer than the preindustrial climate using the pseudo-global warming method. The used data base for future climate is DDS5TK (5km-grid Dynamical Downscaling Dataset, SI-CAT DDS5TK [3]).

Here we have estimated the global warming effects between current and future climate on the summer in the past 10 years of 2010 to 2019. In these ten years, both the rainy-cool and hot summers are included. The area is the southern part of Kanto area in Japan.

The highly resolved results show the regional features, e.g., as follows:
The increases of the one-month averaged temperature (Tave) is larger in the coastal area within about 1-km than those in the inland area. This is because the temperature of sea-breeze becomes higher in the future climate.
The increase of "Tave" in the valley bottom area is also larger than the hill top. This is also related with the wind speed. It is also observed that the temperature increase depends on the shape of the valley, those are, depth (~tens of meters), width (~hundreds of meters) and the mouth of the valley. The temperature increase is larger for the valleys with the mouths facing to the coastal side.
These results can contribute to the planning of sustainable future cities by local governments and area managers.

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Impact of Drone Observation on Micrometeorology Predictions

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Key Words: *Mircrometeorology simulation, Drone logistics, Long Short-Term Memory*

In future urban cities, various autonomous systems will provide various social services accounting the ever-changing and complex weather and society without people's awareness. The autonomous systems will be connected to the Internet and constantly access integrated information on past, present, and future weather and social networks reproduced in cyberspace. While the autonomous systems providing the services, their real-time sensing data will be assimilated into weather forecasting simulations. That is, the so-called digital twin is achieved through the autonomous systems. The use of the real-time sensing data for weather predictions is the key to realize such future cities. One of the promising future social services is the drone logistics, which is expected to start in urban areas where people and goods are concentrated. Drones rely on the micrometeorology (microscale weather near the surface) rather than the meteorology. Their sensing data would be useful for the micrometeorology predictions. We here aim to confirm the impact of real-time sensing data obtained by drones on the micrometeorology predictions. We performed micrometeorology simulations targeting actual urban streets using a multiscale weather model named MSSG (Multi-Scale Simulator for the Geoenvironment [1,2]). Obtained dataset were considered as the ground truth and virtual observations were created from the dataset. Prediction tests were then performed using the Long Short-Term Memory (LSTM) of Recurrent Neural Network [3]. We have confirmed that the prediction accuracy is improved by considering the additional information at drone flight altitudes compared with the case in which only the observation data near the ground surface are considered. This indicates a promising future cooperative development of drone logistics and urban micrometeorology predictions.

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Model Intercomparison Study of Jet in Cross Flow for Prediction of Hot Air Recirculation

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Key Words: *Hot Air Recirculation (HAR), Jet in Cross Flow (JICF), LES, POD*

Air-Cooled Heat Exchangers (ACHEs) are large fans sitting atop of high pipe racks in the Liquefied Natural Gas (LNG) plants and discharge a large amount of hot air into atmosphere. The performance of ACHEs can be significantly reduced as the hot exhaust air recirculates back into the ACHEs intakes under crosswind conditions causing the Hot Air Recirculation (HAR). The flow pattern of the hot air discharged from a single ACHE fan under the crosswind condition is similar to a jet in cross flow (JICF). The understanding of the physics in JICF will therefore help predict HAR phenomena for achieving more efficient operations and production increase of LNG plant.

This study aims to clarify the physics in JICF by means of three different numerical approaches (1) steady flow simulation with the Reynolds-Averaged Navier-Stokes (RANS) model, (2) Large Eddy Simulation (LES) and (3) Direct Numerical Simulation (DNS). The computational conditions in Sherif et al (1989) [1] and Yuan et al (1999) [2] were adopted, but with various grid settings. The same coarse-resolution uniform grid was used for the three different LES models; implicit LES [3], front-flow/red (FFR) [4] and MSSG [5], and RANS models with different schemes. The results were compared with the reference high-resolution DNS results.

The three LES models reproduced the mean and fluctuations of velocity magnitude well, while the RANS models did not reproduce the fluctuations successfully although the mean velocities were reproduced well. The coarse-uniform-grid simulations show similar flow profiles with the DNS although they fail in reproducing the turbulence generation near the jet outlet. In order to clarify which modes of flow were captured and missed in the coarse simulations, the Proper Orthogonal Decomposition (POD) analysis was applied to 2D snapshots of the simulation results. The analysis provides physical insight into the relation between the grid resolution and flow modes in JICF, which will contribute to predicting HAR phenomena.

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Sensitivity Study of Turbulence Models and Mesh Size for CFD Simulations of Jet in Cross Flow for Prediction of Hot Air Recirculation

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Key Words: *Jet in cross flow, Large eddy simulation, Unsteady Reynolds-averaged Navier-Stokes*

In the liquefied natural gas (LNG) plants, air-cooled heat exchangers (ACHEs) with an array of large fans are utilized to cool hot process fluid, and hence, a large amount of hot air is emitted into atmosphere. The performance of ACHEs can be reduced remarkably if the hot exhaust air recirculates back into the intakes of ACHEs under crosswind condition, which is so called hot air recirculation (HAR). The flow pattern of the hot air discharged from a single ACHE fan under the crosswind condition is analogous to a jet in cross flow (JICF). Therefore, it is considered that the understanding of flow behavior in JICF is helpful for predicting HAR phenomena to improve the operations of LNG plant and increase its production.

The present study aims to investigate the effects of turbulence model and mesh size on CFD simulation results of JICF. The computational conditions used is the same as those in Sherif et al. [1] and Yuan et al. [2]. CFD simulations were conducted using large eddy simulation (LES) and unsteady Reynolds-averaged Navier-Stokes (URANS) model in the modified open-source CFD code FrontFlow/Red (FFR) [3]. The turbulence models for LES and URANS are dynamic Smagorinsky model (DSM) [3] and realizable k-epsilon (RKE) model [4], respectively.

The DSM-based LES analyses predicted the mean and fluctuations of velocity magnitude well for both coarse mesh and fine mesh, compared with the experimental results by Sherif et al. [1] and LES analysis results by Yuan et al. [2]. On the other hand, the RKE-based URANS simulations underpredicted the fluctuations remarkably although the mean velocities were predicted relatively well for both coarse mesh and fine mesh. Also, fine mesh provided better predictions of the mean and fluctuations of velocity magnitude than coarse mesh for both LES and URANS simulations. The difference between LES and URANS simulation results is attributed to the fact that the DSM model for LES can predict the sub-grid scale (SGS) turbulent eddy viscosity better, and however, the RKE model in URANS overpredicted the turbulent eddy viscosity and hence the predicted flow fluctuations are damped by the numerically overestimated turbulent diffusion.

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Three-Dimensional Super-Resolution of Passive-Scalar and Velocity Distributions Using Neural Networks for Real-Time Prediction of Urban Micrometeorology

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Key Words: *Building-Resolving Micrometeorological Simulations, Three-Dimensional Super-Resolution, Neural Networks, Real-Time Prediction*

In future cities, various IoT devices such as drones will constantly access meteorological data and social network information on cloud networks. Each system using IoT devices will provide a variety of services in response to complex changes in weather and society without people being aware of it. Such social services will require real-time predictions for urban micrometeorology.

Our research group has developed a micrometeorological model that can resolve buildings and tree canopies at several meter resolution in urban areas (e.g., [1]). However, the computational cost of such simulations is high, and the real-time prediction is difficult even with a supercomputer. We have recently proposed a "super-resolution simulation method" [2] using deep learning, where high-resolution inferences are obtained with a neural network from the low-resolution results of micrometeorological simulations. Once the neural network is trained, it can make inferences at low computational cost, which would make the real-time prediction possible.

Our previous study [2] demonstrated the feasibility of super-resolution simulations for two-dimensional temperature, whereas the information of three-dimensional wind velocity is essential for flying IoT devices such as drones. Although there have been studies on super-resolution of three-dimensional velocity with neural networks (e.g., [3]), these studies discussed canonical flows such as channel turbulence and the effectiveness of three-dimensional super-resolution for complex real-world flows has not been confirmed. This research proposes a neural network super-resolving both passive-scalar and three-dimensional velocity and applies it to building-resolving micrometeorological simulations in urban cities. We discuss the generalization performance of the neural network and the feasibility of the real-time prediction using it.

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Combining Artificial Neural Networks and Modal Decomposition Methods to Assess and Forecast Ship Performance in Waves

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Key Words: *Artificial Neural Networks, Dynamic Mode Decomposition, Forecasting*

To ensure the safety of structures, payload, and crew in adverse weather conditions, ships must have good seakeeping and manoeuvrability performance. In this regard, ships must meet International Maritime Organization Guidelines and Regulations and NATO Standardization Agreements. Therefore, the prediction capability of ship performance in waves, along with the understanding of the physics involved, is of utmost importance. Synergic computational and experimental fluid dynamics studies [1] have demonstrated the maturity of computational tools for the prediction of ship performance in waves, including highly nonlinear dynamics in extreme sea conditions. The computational cost associated with the analysis is generally very high, especially if statistical convergence is sought after and complex hydro-structural problems are investigated via high-fidelity solvers. Computations and experiments usually produce a large amount of data, whose investigation via machine learning (ML) methods could shed light onto the underlying physics of the problem. Nevertheless, ML studies for ships in waves are still limited, where ML is usually used as a black box, with limited explanation capabilities.

The objective is to present and discuss the development and application of ML methods to improve knowledge and forecasting of global/local loads, motions, and trajectories for ships operating in waves. Hybridization of ML approaches, such as recurrent neural networks (RNN) [2], with modal-decomposition methods, such as dynamic mode decomposition (DMD) [3], is investigated to (a) predict/forecast global/local loads, motions, and trajectories of ships operating in waves, (b) extract statistical predictive models for relevant dynamics and kinematic quantities of interest, and finally (c) facilitate the interpretation and explanation of ML results.

The proposed hybrid approach is data driven and equation-free, providing also, whenever possible, the uncertainty associated with the prediction. Development, assessment, and optimization of hybrid architectures is discussed for the course keeping of a destroyer-type vessel in stern-quartering irregular waves at sea state 7. Training data are taken from URANS computations in [1]. A first architecture runs in parallel the DMD and RNNs. The final forecast is provided by a Bayesian version of RNNs; DMD is used to gain knowledge of the physics via linear modal representations; finally, the difference between linear (DMD) and nonlinear (RNNs) results is used to assess the importance of the nonlinear dynamics. A second architecture is studied, applying RNNs to the modal coordinates associated to the DMD representation, allowing for equivalent capabilities to the first architecture.

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Domain-Aware Active Learning for Multifidelity Optimization

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Key Words: Multifidelity methods, active learning, Bayesian optimization, multidisciplinary design optimization

Bayesian optimization is a popular strategy for the optimization of black-box objective functions [1]. In many engineering applications, the objective can be evaluated with multiple representations at different levels of fidelity, to enhance a trade-off between cost and accuracy. Accordingly, multifidelity methods have been proposed in a Bayesian framework to efficiently combine information sources, using low-fidelity models to enable the exploration of design alternatives, and improve the accuracy of the solution through limited high-fidelity evaluations [2]. Most multifidelity methods based on active learning search the optimal design considering only the information extracted from the surrogate model. This can preclude the evaluation of promising design configurations that can be captured only including the knowledge of the particular physical phenomena involved [3]. To address this issue, this presentation discusses original domain-aware multifidelity Bayesian frameworks to accelerate design analysis and optimization performances. In particular, our strategy comes with an active learning scheme to adaptively sample the design space, combining statistical data from the surrogate model with physical information from the specific domain. Our formulation introduces physics-informed utility functions as additional contributions to the acquisition functions. This permits to enhance the active learning with a physics-based insight and to realize a form of domain awareness which is beneficial to the efficiency and accuracy of the optimization task. The presentation will discuss several applications and implementations of the proposed approach for single discipline and multidisciplinary aerospace design optimization problems.

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Gaussian process regression for ship dynamics: Between the Scylla of slow Karhunen-Loève convergence and the Charybdis of transient features

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Key Words: Gaussian Process, LAMP, Karhunen-Loève Theorem, Vertical Bending Moment

For a number of stability and fatigue problems in marine structural dynamics, engineers need accurate statistics for kinematic and dynamical quantities, such as pitch angles and bending moments. Unfortunately, the response statistics depend on stochastic processes, such as sea surface elevation, in a relationship with important nonlinearities. These difficulties prevent naval architects and safety engineers from using fast Fourier space methods such as Weiner-Khintchine, and instead force them to perform expensive experiments and time-consuming numerical simulations.

In order to avoid the data requirements in the Monte Carlo regime, we present a machine learning framework to minimize training set requirements. Our framework consists of two parts. First, we use the Karhunen-Loève theorem to represent stochastic sea states over finite intervals with a low dimensional projection that nonetheless captures the features important to hydrodynamics and structural mechanics. However, the choice of interval is caught between the Scylla of slow Karhunen-Loève series convergence for long duration and the Charybdis of transient behavior for small duration. To combat this dilemma, we propose a division into a fixed region, designed for parametric interpolation and machine learning, and a variable region, designed to control transients and initial conditions.

The second part of our framework is a Gaussian Process Regression surrogate model designed to learn the mapping from sea state to structural outputs. The Gaussian Process is able to take advantage of the low dimensional parametric representation of the sea state in order to converge with reasonably-sized training sets (on the order $n \approx 100$). At the same, we use a projection representation in order to directly reconstruct the output time series. The principal advantages of the Gaussian Process surrogate are the blazing speed of evaluation–ten thousand times faster than the Large Amplitude Motions Program we use to generate data [1]–and the built in uncertainty quantification.

Taken together, we can reconstruct the statistics of the responses by sampling sea states via the Karhunen-Loève construction, estimating the corresponding model outputs using the trained Gaussian Process, and estimating statistics of interest through direct Monte Carlo calculation.

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Generalized Neural Network Approach to Ship Motion Forecasting

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Key Words: Ship Hydrodynamics, Maneuvering, Seakeeping, Machine Learning, Neural Networks

Accurate and computationally efficient prediction of ship responses in waves with physics-based numerical hydrodynamic tools is an integral part of the ship design process and in the development of operational guidance for vessels. However, once ships are designed, built, and deployed into the harsh ocean environment, analyses performed for nominal operating and environmental conditions may not reflect the real-time phenomena experienced by the vessel. As autonomy becomes more prominent in deployed vessels, accurate short-term temporal forecasting of ship responses, given the current wave environment and desired ship operation (e.g. speed, heading, maneuver, etc.) can reduce the overall risk on-board both manned and unmanned vessels. Numerical hydrodynamic tools that leverage formulations such as blended-nonlinear potential flow and unsteady Reynolds-averaged Navier-Stokes (URANS) methods, allow for simulations of ship motion in waves with varying levels of fidelity but are too expensive computationally to produce a real-time temporal prediction of ship responses, given the desired operation and the current wave environment. The recent advancements in machine learning and neural networks has led to their consideration for marine dynamics problems, where data produced by higher fidelity numerical tools can be employed to build fast-running surrogates that represent the underlying dynamical process. In particular, long short-term memory (LSTM) neural networks have been utilized for ship motion forecasting and were demonstrated most recently in [1], where a methodology was developed to represent the full six degree-of-freedom (6-DoF) ship response in irregular random waves. Previous methodologies implementing neural networks and ship motions have focused on developing a model based on a single speed, heading, and sea state and have not been shown to be generalizable to other operating and seaway conditions. The current work extends the work developed in [1] into a more generalized framework by using estimates of ship encounter frame and including training data from different sea states. Estimating the encounter frame based on a given nominal speed, heading, and maneuver and considering different sea states will empower the models to be more general in developing a relationship between the instantaneous wave elevation around the hull and the global ship motion response. The present work will detail the improved methodology, demonstrate a case study for a ship in multiple seaway and operating conditions, and explore the convergence of the constructed models with respect to training data quantity.

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Multi-fidelity Bayesian experimental design for extreme-event statistics

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Key Words: *multi-fidelity model, Bayesian experimental design, extreme events*

In this work, we develop a multi-fidelity Bayesian experimental design framework to efficiently quantify the extreme-event statistics of an input-to-response (ItR) system with given input probability and expensive function evaluations. The key idea here is to leverage low-fidelity samples whose responses can be computed at a certain fraction of that for high-fidelity samples, in an optimized configuration to reduce the total computational cost. To accomplish this goal, we employ a multi-fidelity Gaussian process as the surrogate model of the ItR function, and develop a new acquisition model based on which the optimized next sample can be selected in terms of its location in the sample space and fidelity level. In addition, we develop an inexpensive analytical evaluation of the acquisition model, avoiding numerical integrations that are prohibited for high-dimensional problems. The new method is tested in the context of bi-fidelity models for a series of synthetic problems with varying dimensions, low-fidelity model accuracy and computational costs. Comparing with single-fidelity method and bi-fidelity method with a pre-defined fidelity hierarchy, our method consistently shows best (or among the best) performance for all the test cases. Finally, we demonstrate the superiority of our method in solving an engineering problem of estimating the extreme ship motion statistics in irregular waves, using computational fluid dynamics (CFD) with two different grid resolutions as the high and low fidelity models.

Power Spectrum Estimation Based on the Long and Short-Term Memory Neural Network Subject to Missing Data

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Key Words: *Neural network; Stochastic process; Missing data; Power spectrum*

Abstract: This paper develops a power spectrum estimation method based on long short-term memory (LSTM) neural network subject to the missing data[1]-[2]. In actual engineering applications, the accuracy of power spectrum increases with the rise of time history samples.. However, there are some cases where the data is difficult to obtain or some data may be missing, due to the restrictions of the measurements or data corruption. In this regard, LSTM neural network is introduced to deal with the missing data problem. First, missing data can be filled with zeros to obtain samples of the full time history. In order to solve the problem of exploding and vanishing gradients occurring in neural networks, LSTM blocks are used to embed gates into hidden neurons of recurrent neural networks. In this sense, an advantage of the LSTM framework is that key information can be stored or updated by manipulating the gates introduced. Furthermore, LSTM models are able to retain information for a long time without vanishing gradients. In addition, the zero padding samples are used to train the LSTM neural network model. The accuracy of the model can be improved by appropriately selecting an prediction sequence length and building the corresponding neural network structure. Next, the trained LSTM neural network model can be used to predict the remaining missing data and obtain the power spectrum. During the forecasting process, the predicted value is used to replace the zero value, and the sample time series data is continuously updated until all the zero values are replaced by the predicts of the neural network model.The significant advantage of this method is that it can maximize the use of missing data to obtain more time history samples, so that the target power spectrum can be restored more accurately[3]. The comparison between the target power spectrum and the power spectrum estimation based on LSTM neural network demonstrates the accuracy and effectiveness of the proposed method.

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Predicting failures from data and physics: a nearly-real-time approach to system prognostics

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Key Words: Prognostics and Health Management, Remaining Useful Life, Multifidelity Modeling, Machine Learning

The fault detection and failure prognosis of complex engineering systems are a major challenge for health management and maintenance planning, as the mutual interactions of heterogeneous subsystems result in behaviours that are difficult to model accurately. A robust real-time estimate of the current system health and Remaining Useful Life (RUL) is a key element to enable the actuation of predictive maintenance tasks and reduce the overall operating costs of the equipment. At the same time, the high computational cost usually associated to such estimates hinders the execution of these tasks on-board [1]. We propose to combine physics-based representations with data driven knowledge of the observed system, to achieve accurate estimations of the current and future health of the monitored equipment, while keeping the computational time of the entire process suitable for a nearly-real-time evaluation [2]. We demonstrate our approach on the failure prognosis of an aircraft electromechanical actuator for secondary flight controls. The results suggest that the algorithm is able to assimilate measured data in real-time, learning from physics to progressively increase the accuracy and robustness of RUL predictions.

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Reduced Operator Inference for Nonlinear Partial Differential Equations

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Key Words: scientific machine learning, operator learning, non-intrusive model reduction, nonlinear partial differential equations, data-driven modeling

We present a new *scientific machine learning* method that learns from data a computationally inexpensive surrogate model for predicting the evolution of a system governed by a time-dependent nonlinear partial differential equation (PDE), an enabling technology for many computational algorithms used in engineering settings. Our formulation generalizes to the PDE setting the *Operator Inference* method previously developed in [B. Peherstorfer and K. Willcox, *Data-driven operator inference for non-intrusive projection-based model reduction*, Computer Methods in Applied Mechanics and Engineering, 306 (2016)] for systems governed by ordinary differential equations. The method brings together two main elements. First, ideas from projection-based model reduction are used to explicitly parametrize the learned model by low-dimensional polynomial operators which reflect the known form of the governing PDE. Second, supervised machine learning tools are used to infer from data the reduced operators of this physics-informed parametrization. For systems whose governing PDEs contain more general (non-polynomial) nonlinearities, the learned model performance can be improved through the use of *lifting* variable transformations, which expose polynomial structure in the PDE. The proposed method is demonstrated on a three-dimensional combustion simulation with over 18 million degrees of freedom, for which the learned reduced models achieve accurate predictions with a dimension reduction of six orders of magnitude and model runtime reduction of 5-6 orders of magnitude.

A Hierarchical Design on Bioinspired Structural Composites using Reinforcement Learning

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Key Words: *Biologically inspired structural composite materials, reinforcement learning, optimization, Q learning, hierarchical design, design system*

Here we propose a new design method using reinforcement learning to solve bioinspired composite materials in a complex system. Biological structural materials are made by a stiff matrix and a compliance glue to exhibit extraordinary mechanical properties which synthetic materials do not possess. The reason for this excellent performance is because a particular order makes them of microstructures. To imitate the exceptional material properties of biomaterials, the idea of bioinspired structural material has been proposed. However, the number of combinations of design space is usually intractable. Therefore, we offer a new design method by using reinforcement learning to solve the problem. Here we developed a hierarchical design paradigm. The hierarchical design process starts from a design space with limited combinations. After obtaining the best design of the current system size, we expanded the design system and searched for the best design with higher resolution. We searched for the best crack resistance by using the hierarchical reinforcement learning from a lower resolution. By comparing the design results in the two design systems, the hierarchical design can effectively increase the convergence rate. We further discussed the results obtained from each hierarchical level. It can be observed that the best structure obtained from a high-resolution design space shows a significant improvement by depressing the stress concentration at the crack tip. The best composition was examined through 3D printing. The experimental results show that there is an excellent agreement with our AI design. The design framework proposed in this research can be used as an alternative method for optimization in a complex design system with various constraints. This research can be potentially applied to bionic structural design, nanoengineering, and material design in the future.

A Neural Network Enhanced Finite Element Method for TPMS based Mechanical Metamaterials Simulation

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Key Words: *Machine Learning, Neural Network, RVE, Finite Element Method, Triply Periodic Minimal Surface*

Mechanical metamaterials are artificial structures where the structure rather than the composition primarily determine their material properties. Triply periodic minimal surface (TPMS) is one of the well-known metamaterials; its volume is occupied with distorted morphology and sophisticated tunnel systems. Such distinctive topology-driven cellular structures can also be discovered in nature, such as butterfly wings and sea urchins [1]. In tradition, the finite element method (FEM) is employed to simulate the metamaterials, but plenty of defects and twist geometry pose difficulty in the model construction. Excessive low-quality mesh is found in the TPMS model, and therefore, the direct numerical simulation (DNS) becomes computationally inefficient and ineffective. In this study, we employ the neural network enhanced finite element method (NN-FEM) to improve the simulation performance. In this framework, a surrogate model can be employed without detailed structural topologies, and the hypothesis constructed by the neural network replaces the traditional analytical constitutive model in the numerical simulation. In order to train the neural network offline, the representative volumetric element (RVE) is defined at a local scale, and its mechanical responses are obtained by imposing various boundary conditions [2] to acquire the datasets. The usage of RVE in the surrogate model results in a homogeneous mesh to model a complicated TPMS structure. Such simple mesh not only saves the unfavorable mesh cost, but also enhances the convergence of the solver, which further saves computational costs. Some comparisons with traditional FEM are performed to validate the superior efficiency of NN-FEM. Dataset tuning methodologies and generalized-TPMS scheme are also proposed to speed up the NN-FEM, which will be presented. TPMS structure will be parameterized, and thus regarded as input of neural network in NN-FEM. Various engineering applications have been examined and the numerical results in both deformation and stress distribution is consistent with DNS results, which verify the robustness and effectiveness of the framework toward TPMS. The scheme provides a new and efficient way to design, model, and optimize complicated engineering metamaterials.

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A new Physics-Informed Neural Network based Topology Optimization framework for structural optimization

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Keywords: Topology optimization, Evolutionary structural optimization, Physics informed neural network, Machine learning, Solid Mechanics.

This paper presents a novel paradigm for Physics-Informed Neural Network based Topology Optimization (PINNTO). The proposed study replaces conventional FEA with an energy-based PINN to establish an approximation function for the displacement field [1]. Here, a supervised neural network that respects governing energy method described by partial differential equation (PDE) is trained without any labelled data to solve linear elastic solid mechanics problems. Combining with Bi-directional Evolutionary Structural Optimization (BESO) as the generation of solid-void optimal topology, a new PINN based topology optimization is developed in this paper [2]. A number of compliance minimization examples are presented to demonstrate the validity and effectiveness of the proposed PINNTO for achieving convergent optimal designs for structures. Compared with the existing BESO method, PINNTO does not require traditional FEA. Instead, the structures obtained using PINNTO is comparable to the conventional topology optimization methods.

Keywords: Topology optimization, Evolutionary structural optimization, Physics informed neural network, Machine learning, Solid Mechanics.

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A Novel Coarse-Grained Model for Chloride Effect on Glass Reinforced Polymer Composites

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Key Words: *Molecular dynamics, Coarse-grained model, Glass fiber, Composites, Chloride*

Glass fiber reinforced polymers (GFRPs) have been widely utilized in marine applications due to its inexpensive, versatile and excellent performance. In the past decade, extensive experimental and theoretical studies have been conducted on reinforced polymer composites to facilitate the development of construction materials. Although a number of experimental investigations have been carried out to determine the characteristics of GFRPs under various experiments, the in-depth insight into molecular-scale processes involving interfacial interactions between fiber and matrix cannot be provided. Therefore, molecular dynamics (MD) simulation is needed when analyzing the mechanism of material failure that is originated from molecules. Despite the wide application of MD simulation in the modeling of GFRP, its applicability is limited by the tremendous computational resources and the restricted time and spatial scale compared to experiments. To bridge nanoscale modeling and macroscopic experiment, coarse-grained (CG) models beyond the capacity of atomistic simulations have been put forward. In this work, a CG model of GFRP is developed, the applicability and efficiency of which in predicting GFRP composites under environmental-introduced deterioration are evaluated through verification processes. The developed model consists of defining CG beads for the microscopic system and calculating their spatial distribution. The interactions between beads are then obtained based on the results from full atomistic models. To predict mechanical behaviors of GFRP under marine environment, the degradation of GFRP caused by chloride effect and the mechanism involving bond breaking and formation are explored. The CG model can reproduce macroscopic experimental observations and measurements. Tensile fracture snapshot of CG model is compared with SEM photo of GFRP composite, also the morphologies of the CG models that present the deterioration of GFRP under chloride effects are compared. The application of the method in modeling of large unit cells with randomly distributed glass reinforcements is examined. The changes of internal pore distribution, interfacial morphologies, and the mechanical properties of GFRP show that the degradation of microstructure and mechanical properties under environmental intervention can be well predicted by this novel CG model. The newly proposed modeling framework with basic description of material structure can be further extended to the research on the deterioration of other engineering composite materials, and provide insight towards the development of new nanocomposites.

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Artificial Neural Network Potential Model for Pb-Te-Ga Alloy Materials

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Key Words: *Artificial neural network, Potential energy and force, Thermoelectric materials, Pb-Te-Ga alloy materials, First-principles calculation*

Lead telluride (PbTe) emerged as a promising thermoelectric material for intermediate-temperature waste-heat-energy harvesting. For the purpose of increasing its ZT value and further reducing its thermal conductivity, it can be achieved by doping Ga[1]. However, since the optimal composition of the complex and diverse ternary material, PbTeGa, has not yet been discovered, numerical calculations can be used to accelerate the exploration. The thermal conductivity coefficient of Ga ternary thermoelectric materials with different compositions can be calculated using well-known numerical methods of Equilibrium and Non-Equilibrium Molecular Dynamics (EMD and NEMD, respectively). Yet, there is no complete and reliable material potential function in the literature to accurately describe the interatomic interactions in ternary thermoelectric materials. Therefore, in this work, we use an artificial neural network (ANN) to fit the potential energy of binary and ternary thermoelectric materials. Firstly, the neural network potential package (n2p2) program[2] was used to fit the potential function of the binary material PbTe with the training dataset of 12,300 PbTe structures generated by first-principles calculations. Then, the function was used to perform molecular dynamics (MD) simulations. As a result, the verified microstructure is stable and the lattice volume energy curve is consistent with the first-principles calculations. Furthermore, in the prediction of material-related properties, taking elastic modulus as an example, the error between the predicted value and theoretical value provided by Material Project is within 6%. This shows that ANNs can successfully and effectively predict the potential energy and force of the binary material through the characteristics of the local atomic environment. Secondly, the research is further extended to the ternary thermoelectric material PbTeGa, the training dataset contains 24,600 PbTeGa structures, and a special step-by-step training strategy is proposed, in which the potential functions of pure element, binary and ternary materials are fitted separately. The advantage of the strategy is that the accuracy of potential energy fitting of ternary materials can be imporved and guided by the fitted parameters of existing pure elements and binary materials. In summary, the potential functions fitted by ANNs are efficient, accurate, and not affected by the scale of the system. The present work results are expected to be helpful for the development of PbTeGa ternary thermoelectric materials.

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Bio-inspired, Machine Learning-designed/optimized Metastructures and Composites with Synergistic Mechanical Properties

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Key Words: *Instructions, Multiphysics Problems, Industrial Applications, Covid-19*

Natural materials, which have risen from billions of years of evolution, have developed unique characteristics, such as hierarchical structures, multi-functionality, self-assembly at ambient temperature and pressure, capabilities of self-healing and environmental adaptation. Distinct from engineering materials, which are unable to perform both lightweight and high strength; high stiffness and high toughness, biological materials are often composites of hard/brittle minerals and soft/ductile proteins arranged into complex hierarchical structures which possess remarkable mechanical properties, combining lightweight, high strength and high toughness owing to strengthening and toughening mechanisms from nano-, micro-, meso-, and macro-scales.[1] Learning from Nature can lead to revolutionary breakthrough and innovation in materials science and technology. In this talk, selected biological materials, including abalone nacre, dragonfly wings, bamboos and plant seeds will be introduced. [2,3] Inspired from the structural designs of these natural materials, we further applied multi-scale simulation/modelling, genetic algorithm, machine learning, and A.I.-related approaches to optimize the bio-inspired structures and validated by 3D printing and mechanical testing. Novel mechanical metastructures and composites inspired from Nature and optimized by A.I. could lead to wide potential applications in industrial fields, including bicycles, automobiles, aerospace, intelligent robots, biomedical materials and assistive devices.

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Database-Driven Multiscale Simulation of Inelastic Materials through an Efficient On-the-fly Generation of Data

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Key Words: *Multiscale Simulation, Data-Driven Computational Mechanics, Deep Material Network*

Due to many challenges posed by traditional multiscale simulation methods, there has been lately an increasing interest in data-driven multiscale tools. For instance, inspired by DDCM [1], Xu et al. [2] proposed a data-driven FE^2 solver in which online macroscopic analysis is performed by searching over an offline-generated database of stress-strain points. Although the results were promising, this approach has its limitations: it requires a fixed and large dataset, hence making it not suitable to problems with path-dependent mechanical response. It is also computationally expensive, although to a lesser extent than the traditional methods. In this work, we combine DDCM with a deep material network (DMN) [3] to formulate a DMN-DDCM solver to circumvent those difficulties in data-driven multiscale simulation (DDMS). By utilizing a multi-level strain sampling strategy whereby the range of data is adaptively adjusted, we can timely feed DDCM with sparse, dynamic datasets generated through DMN. This strategy greatly enhances efficiency of DDMS. The on-the-fly generation of data is guided by macroscopic stress-strain conditions and DMN which enables the flow of information between scales through homogenization/de-homogenization and can capture complex materials behaviors. The result is a data-driven multiscale solver which can both efficiently and accurately capture the intricate responses of heterogeneous materials. This solver shows the potential to become an excellent and reliable tool in data-driven multiscale simulation.

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Deep neural network battery life and voltage prediction by using data of one cycle only

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Key Words: *Deep neural network, LiFePO4/graphite cells, End-of-life, Remaining useful life, Data-driven features*

Rechargeable batteries, such as LiFePO4/graphite cells, have great economic and environmental value. In this work, we proposed deep neural networks with a special convolutional training strategy and taking advantage of recently published battery cycling data. The residual life of a battery can be predicted with a mean absolute percentage error of 6.46%, using only one cycle of testing. The cycle-by-cycle profiles, such as discharge voltage, capacity, and power curves of any given cycle, of used batteries with unknown age can also be accurately predicted. Moreover, our models can extract data-driven features from the data which were much more influential on the predicted properties than human-picked features such as the maximum and minimum temperatures, based on the analysis by using deep tayler decomposition. Finally, a powerful Full RUL DNN which allows the prediction of remaining useful life (RUL) and the current battery age of used batteries is proposed. Our DNNs are suitable to be an important component of modern quality control systems in battery manufacturing and battery management systems. It is expected to provide tremendous economic and environmental benefits since reuse and recycling of batteries can be better planned.

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Geometric and Recurrent Neural Network for Surrogate Modelling of Polycrystalline Metals

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Key Words: *graph neural networks, recurrent neural networks, stress-strain evolution, texture evolution, elasto-viscoplasticity, mechanical properties*

Multiscale simulation is widely used in modeling microstructure-induced inelastic mechanical behavior. However, direct numerical simulation (DNS) and concurrent multiscale simulation suffer from an expensive computational cost that makes the process infeasible. In this work, we aim for developing an efficient surrogate model for constitutive modeling of metallic materials that combine graph neural networks (GNN) [1] and recurrent neural network (RNN) [2, 3] to incorporate geometric representation of polycrystals and memory-dependent behavior. Extended from Vlassis et al. [1], we introduce a graph neural network to extract grain topology and properties in polycrystalline metals as low-dimensional graph embedding to predict the evolution of the properties, e.g., texture. By such graph representation, the nature of the polycrystalline materials topology, i.e., grain connectivity, can be incorporated into the machine learning model, and generalized to predict mechanical response of unseen topologies at the online stage. To further enhance the predictability on nonlinear elasto-viscoplasticitic behavior, RNN is incorporated to establish time correlation of the historical loading path. In this work, the proposed hybrid machine learning model is trained on the dataset generated by a high-fidelity crystal plasticity model to predict stress-strain response and microstructure evolution under uniaxial tension and various loading path. The predictions of the proposed surrogate model show a good agreement with DNS method with a significant improvement in computational efficiency. We also demonstrate the generalizability of the proposed surrogate model by verification on various polycrystalline geometries. This work paves the path for future concurrent multiscale simulations, such as macroscopic formability coupling with microscale texture evolution.

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HiDeNN-TD: Reduced-Order Hierarchical Deep Learning Neural Networks

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Key Words: *Hierarchical Deep-learning Neural Networks, Proper Generalized Decomposition, Convergence Study and Error Bound*

We propose a novel reduced order deep learning approach for solving a class of PDEs, called HiDeNN-TD [1], which is a tensor decomposition (TD) [2] based reduced-order model of the hierarchical deep-learning neural networks (HiDeNN) [3]. The proposed method keeps advantages of both HiDeNN and TD methods. HiDeNN-TD adopts the concept of separation of variables and considers the solution of PDEs as a summation of the products of multiple one-dimensional functions. But differently, each of these 1D functions is represented by structured deep neural networks (DNNs), i.e., the 1D HiDeNN. In these neural networks, the weights and biases are functions of the nodal positions, which allows the optimization of the nodal coordinates in each dimension. This idea makes the HiDeNN-TD more accurate than the finite element method (FEM) and conventional proper generalized decomposition (PGD) [4] and TD, using a fraction of the FEM degrees of freedom. Here, the accuracy and convergence of the method have been studied theoretically and numerically, with a comparison to different methods, including FEM, PGD, TD, HiDeNN and Deep Neural Networks. Theoretical analysis and numerical examples both show that HiDeNN-TD has a high accuracy with orders of magnitude fewer degrees of freedom than FEM, which shows a high potential to achieve fast computations with a high level of accuracy for large-size engineering and scientific problems. As a trade-off between accuracy and efficiency, we further propose a highly efficient solution strategy called HiDeNN-PGD. Although the solution is less accurate than HiDeNN-TD, HiDeNN-PGD still provides a higher accuracy than PGD/TD and FEM with only a small amount of additional cost to PGD. In addition, we have theoretically shown that the PGD/TD converges to FEM at increasing modes, and the PGD/TD solution error is a summation of the mesh discretization error and the mode reduction error.

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Intelligent Nonlinear Multiscale Simulation of Injection-Molded Short-Fiber-Reinforced Composites

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Key Words: *Nonlinear Multiscale Simulation, Mechanistic Machine Learning, Fiber-Reinforced Composites, Deep Material Network (DMN), RVE, FEA Software LS-DYNA*

Short-fiber-reinforced composites (SFRC) have been widely used as high-performance engineering materials for structural applications in automotive and electronics industries. Typically, SFRC are manufactured by injection molding, which induces heterogeneous microstructures across different length scales, and the resulting nonlinear anisotropic behaviors are challenging to predict by conventional micromechanical methods. In this work, we present a data-driven multiscale modeling framework that integrates the injection molding simulation, material homogenization, and a mechanistic machine learning model referred to as Deep Material Network (DMN) [1]. The physics-embedded DMN learns the microscale material morphologies hidden in Representative Volume Elements (RVE) [2] of composites through offline training, and the trained network is able to predict the nonlinear material behaviors at a computational speed orders-of-magnitude faster than the high-fidelity RVE simulation. Through transfer learning [3] of different material microstructures, a unified DMN database is created to cover a full range of SFRC geometric descriptors. Recently, we have coupled the trained DMN database with macroscale finite element models in the engineering simulation software LS-DYNA to perform concurrent multiscale structural simulations [4]. The proposed multiscale simulation framework achieves extraordinary computational performance, and it is quite promising for the design and analysis of composite structures.

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Inverse Design of Face-Like 3D Surfaces via Deep Learning

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Key Words: *4D printing, Shape morphing, Inverse design, Deep learning, Fully Convolutional Network, Finite element analysis (FEA)*

4D printing is an extension of 3D printing technology. By printing smart materials, 3D-printed objects have the ability to deform again due to certain external stimuli such as heat. Although the shape morphing characteristics makes it possible to create complex 3D surfaces from 2D simple structures[1], it is very difficult to inverse design this process because of the nonlinearity of the morphing mechanism and the entanglement between different parts. In this study, we use deep learning techniques to overcome this difficulty and automate the inverse design process. Specifically, this research studies a 2D grid design space that deforms to 3D gridshell through 4D printing process. The 2D grid is composed of rectangular arranged double-layered segments. Each layer is made of shape memory polymer (SMP55) or PLA, resulting in four combinations for each segment. The size and material combination of each 2D grid is specified to control both global and local curvatures of the deformed gridshell which can achieve a variety of complex structures. Three traditional Japanese “Noh masks” are chosen as the target shapes because Noh masks are an ideal model system as each mask has unique aesthetic features. We use parametric polynomial functions describe face features and generate random mask designs. Combining with the deformed shapes simulated by FEM software, we produced a dataset which contained 60k data. We use fully convolutional network (FCN) [2] which typically used in image segmentation task to inverse design 2D grids based on the depth images of the desire shapes. The trained FCN model can predicted 2D grid designs with over 0.95 pixel accuracy and 0.9 mean IOU. Also by the calculation of structural similarity, the average similarity of 3D gridshells deformed from FCN-output designs and target 3D gridshells is 0.9. Although the model is limited to the distribution of the training dataset and performs poorly on Noh masks, it is still a successful proof of concept that deep learning can be utilized in the inverse design problem of 4D printing 2D grid design.

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Machine Learning-Based Energy Model and Mechanical Properties of Chemically Complex Ultraelastic High Entropy Alloys

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Key Words: *Atomistic Simulation, Machine Learning, High Entropy Alloy*

The increasing demands for developing novel chemically complex alloys has imposed a significant challenge to the modeling and simulation community. The mechanical properties of these complex alloys are pivotal for their applications; however, the length scale required for studying the plasticity of these alloys is beyond the reach of conventional quantum chemistry calculations. In this study, we harnessed the power of machine learning and trained a potential model for the chemically complex $Ni_{0.25}Co_{0.25}(Hf_{0.33}Ti_{0.33}Zr_{0.33})_{0.5}$ alloy system by combining the spectral neighbor analysis (SNAP) model and the Bayesian optimization based on a large data set of training images labeled with energies and atomic forces computed from the density functional theory (DFT). We demonstrate that the trained potential model can predict the energies and atomic forces of this chemically-complex alloy with high fidelity to the DFT calculations. A series of large-scale (over 10^5 atoms) molecular dynamics simulations were performed to examine the deformation and dislocation dynamics of both nanowires and bulk structures, and the formation of amorphous, shear band-like region following dislocation pinning was observed, which is in excellent agreement with experiments. Furthermore, the large-scale molecular dynamics also revealed the impacts of chemical microenvironment on the dislocation dynamics, which is impossible to be retrieved from current experimental techniques. Hence, the present study demonstrate that the machine-learned SNAP model yields quantum accuracy even for complex alloy comprised of five constituents, allowing for investigating the plasticity deformation of chemically complex alloys with atomistic insights.

Prediction of Wood Surface Characteristics by Using Deep Learning on Tracheid Effect

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Key Words: *Tracheid Effect, Surface Characteristics, Artificial Intelligence, Deep Learning*

Tracheid effect is a phenomenon that a laser speckle appears on the wood surface where the laser light is illuminated on. Recently, based on the tracheid effect, a three-dimensional fiber orientation scanning system (3D FOSS) was developed at the National Tsing Hua University in Taiwan [1]. In contrast to the elliptical shape of the laser speckle formed when the light is irradiated on the surface of the clear wood, non-elliptical shape scattered image is produced when the light is projected on the surface defect (e.g. knot, crack, edge, etc.). To reduce the influence of wood surface defects on the accuracy of fiber direction measurement based on tracheid effect, artificial intelligence (AI) deep learning method was employed to identify the laser speckle.

In this paper, 26234 laser speckle images of Japanese cedar were collected by the 3D FOSS and a database was established. The images were classified into four categories: clear wood, knot, crack, and edge. The You Only Look Once (YOLO) [2], a single-stage object detection algorithm, was used to perform deep learning on the four categories of laser speckle to form a prediction model. YOLO has the advantage of being able to quickly predict and classify the input data with good accuracy. YOLO has been used to perform prediction behaviours such as vegetable and fruit discrimination at different maturity stages [3], flower species discrimination [4] and animal face expression discrimination [5] with accuracy from 80% ~ 90%.

By using the commercially available software package MATLAB, the predicted results can be visualized for comparison with the original specimens. The preliminary results showed that the surface characteristics of the wood can be successfully predicted.

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Surrogates of Crystal Plasticity Models Using Self-Consistent Recurrent Neural Networks

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Key Words: *Plasticity, Surrogate models, Recurrent Neural Networks*

Multiscale approaches are an essential tool of mechanical modeling. From a description of a material's microstructure, and mechanical models of its constituents, the material's effective behavior can be deduced via numerical homogenization. However, leveraging this microstructural knowledge on large-scale components either directly or even using FE^2 approaches can remain computationally prohibitive. A numerically advantageous alternative consists in constructing a surrogate model of the homogenized response, i.e. a faster algorithm that approximates the homogenized response, for example by constructing a Reduced Order Model.

Recently, an alternative approach based on deep-learning algorithms called Recurrent Neural Networks (RNNs) has emerged. A number of studies have established that, given sequences representative of strain histories and the corresponding stress response of various materials, RNN models could be trained to reproduce this behavior.

Unfortunately, the stress response predicted by typical RNN models (based on LSTMs or GRUs) depends on the number of increments used to discretize a given strain-path, leading to poor predictions when long sequences are considered. This shortcoming complicates the application of RNN models to explicit finite element simulations.

The authors have recently proposed an alternative RNN formulation, called Linearized Minimal State Cell or LMSC, that addresses this issue [1]. By updating the RNN's state-variables following exponential decay trajectories, the RNN's response can be made insensitive to the number of increments used to describe a path. As a result, models trained on sequences a thousand long or less can be implemented into explicit finite element frameworks and deliver precise responses for structural simulations involving millions of time-increments.

In this presentation, we will detail applications of LMSCs to elastoplastic models, in particular to homogenized behavior drawn from crystal plasticity simulations. We will discuss the precision of the results and their sensitivity to dataset properties. We will also highlight that directly implementing the RNN-models as finite element material models leads to numerical instabilities, and propose numerical strategies to overcome this shortcoming.

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Topological Optimization of the Dental Implant by Genetic Algorithm and Deep Learning Network

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Key Words: *Dental implant, Topological optimization, Genetic algorithm, Finite element analysis, Mechano-regulatory, tissue differentiation, Deep Learning*

The geometries of dental implants have a great influence on osseointegration and bone healing. Thus, topological optimization of dental implants has been widely discussed in clinical researches. However, the finite element analysis process of osseointegration based on mechano-regulation method [1] is time-consuming. In this study, a genetic algorithm combined with a deep learning network [2] is developed for topological optimization. The deep learning network which can be a substitute for finite element analysis is developed. It can rapidly predict the tissue differentiation in different designs of healing chambers during the bone healing process. The results of osseointegration is evaluated by bone area (BA) and bone-implant contact (BIC) around the implant. In genetic algorithm [3] , the candidate of dental implant is represented as chromosomes via the encoding method. The BA and BIC values are regarded as the fitness function of genetic algorithm.

After several iterations in genetic algorithm, the optimized geometry design of dental implant is obtained. Where the optimized geometry has finer thread at the top and wider space between threads at the middle, which is very similar to the design of the commercial dental implant. Thus, by assigning different constraints or requirements, the current framework can rapidly optimize the design of dental implants to result in the best osseointegration around the implants.

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Unified unit-cell micromechanics model for effective mechanical properties of particulate, fibrous, and laminated composite materials

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Abstract:

This talk presents a new micromechanics model, dubbed unified unit-cell model, to modeling the effective mechanical properties of particulate, fibrous, and laminated composite materials. Composite connectivities are limited to 0-3, 1-3 and 2-2 types, and mechanical properties are limited to linear elasticity. Considering a periodic composite, a representative volume element can be identified as a unit cell. It is divided into only four subcells. This innovative architecture of a unit cell achieves a concurrent simulation of 0-3, 1-3 and 2-2 composite materials by employing the minimum number of subcells among existing unit cell-based micromechanics models. Effective mechanical constants are derived via concentration-factor tensor technique that addresses the micromechanical relations based on the continuity conditions among the unit cell and its subcells. The unified unit-cell micromechanics model retains an explicit formulation for the overall mechanical properties. Numerical results for 0-3, 1-3 and 2-2 composite materials are shown in order to demonstrate the comparability of the present model with the Mori-Tanaka micromechanics model. Moreover, the predictions are compared in view of existing experimental data of particulate composite materials.

A Physics-Informed Machine Learning Meshfree Method for Hydrodynamics Modelling

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Key Words: *Physics-Informed Machine Learning, Hydrodynamics modelling, Meshfree method*

In recent years, machine learning techniques have brought revolutionary changes for hydrodynamics modelling [1]. Herein, a Physics-Informed Machine Learning (PIML) meshfree method for hydrodynamics modelling has been proposed [2]. In the method, the Feedforward Neural Network (FNN) is applied to predict the field variables within the computational domain. The FNN is trained by physics information in terms of the governing equations and experimental observation data. Both explicit and implicit Runge-Kutta (RK) algorithms are leveraged for accurate temporal integration. The performance of the proposed PIML meshfree method has been investigated through benchmark cases. It has proven that the proposed method can effectively simulate hydrodynamics problems with free surfaces. We also highlight that the issue of treating highly uneven particle distributions, which limits the traditional meshfree methods, is greatly alleviated for the proposed PIML meshfree method [2].

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Adversarial Neural Networks for solving variationally formulated Partial Differential Equations

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Key Words: Adversarial Neural Networks, Partial Differential Equations, Variational Formulation

Solving Partial Differential Equations (PDEs) has been a long-standing challenge in numerical analysis, engineering, and computation. Traditional numerical methods have been widely developed and studied in the last decades for this purpose. For example, Galerkin methods seek the solution in a trial space and employ multiple test functions. In these methods, we want to minimize the residual operator in the dual norm of the test space, which equivalenty reformulates as a min-max problem, where the minimization takes place over the trial space and the maximization over the test space [1].

However, Neural Networks have demonstrated their great capacity for solving PDEs as well as nonlinear formulations. In particular, [2] and [3] propose to solve a weak formulation setting combining two networks adversarially as described above: one to approximate the trial solution, and another one for approximating the test maximizer. However, they select suboptimal norms for the optimization.

In our work, we revisit the Weak Adversarial Networks [2, 3], study their features and limitations, and derive related and more robust methods employing Neural Networks. In particular, we propose a nested double Ritz Method: the outer-loop approximates the trial solution, while the inner-loop approximates locally the trial-to-test operator that maps every trial function with its corresponding optimal test function. In addition, we extend the weak formulations to strong and ultra-weak formulations. We show several 1D and 2D numerical results comparing and analyzing these methods.

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AI-driven Photo-based Prediction of Orthodontic Force and Moment under Treatment

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Key Words: *Orthodontics, Artificial Intelligence, Force and Moment Prediction, V-bend Wire*

Evaluation of orthodontic force and moment is essential to establish effective orthodontic treatment. However, the measurement of the force and the moment is difficult under treatment. This study proposes a method to predict the force and the moment from a wire shape using machine learning and the finite element method. The study focuses on the v-bend wire, which is a wire with a v-shaped bend. In order to achieve the above goal, we tried

- Development of a finite element simulation for force and moment evaluation of a V-bend wire
- Generation of training data of AI is generated by the developed finite element method.
- Development of AI for orthodontic force and moment prediction from wire shape.

Application of Self-Organizing Map (SOM) to the Classification of Athletes' Psychological Ability

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Key Words: *Self-Organizing Map (SOM), Psychological ability*

In the field of sports, it is important to improve mind, technique, and physical strength. To give full play to athletes' ability in the competition, we should consider the combination of mind, technology, and physical strength. Technique plays a role based on physical strength, which is dominated by mind. The exertion of psychological level is an important factor for winning the competition. Therefore, it is very important to support athletes from the field of psychology as well.
There are individual differences in psychological competitive ability. Especially in the case of group competitions, understanding the psychological characteristics of individual athletes leads to improvement in team performance. In this research, we use the self-organizing map (SOM) [1] to analyze the athlete's psychological characteristics. Athletes were examined using the Diagnostic Inventory of Psychological Competitive Ability for Athletes (DIPCA.3), the Athletic Coping Skills Inventory (ACSI), the Mental Toughness Index (MTI), and the Sukumune-Hiew Resilience Test (S-HRS). Total scores for each questionnaire were used as the SOM's input data. The results showed that the SOM clustered the athletes according to their psychological ability. Similar athletes with psychological ability were mapped near and clustered into the same group. We confirmed that SOM is a very effective analysis method for the field of sports psychology.

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Automatic Visualization of Various Flow Fields Using Self-Organizing Map

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Key Words: Flow Visualization, Computational Fluid Dynamics, Self-Organizing Map, Machine Learning

The authors had proposed a new visualization method using self-organizing map (SOM) for computed results of fluid flow at the last WCCM conference[1]. Most of existing visualization method gives color depending on a certain physical value, such as pressure, vorticity, etc. However the choice of the physical value is arbitrary and sometimes loses important features. The proposed method firstly classifies all flow properties, i.e. pressure, velocity components and their spatial gradients etc. at each grid point, by giving these properties as high order vectors to SOM. Then color is given to each grid point based on its location on the map so that the flow field be naturally painted including all flow properties. SOM is originally a two-dimensional (2D) map as the main purpose of SOM is to visualize high order vectors, but in the proposed method, the map is not directly viewed and only used to determine color of each grid point. Hence three-dimensional (3D) SOM has been also generated to give three color components based on the map. In the present paper, the proposed method is further investigated to show its capability and validity with various flow fields, such as compressible / incompressible flows. Also the choice of flow properties given to SOM are examined. For instance, only the primitive variables are used, only the spatial gradients are adopted, the second derivatives are included, etc. The results will be included in the extended abstract and be presented at the conference as well.

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Construction of a surrogate model for crash box corruption

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Key Words: *Machine learning, deep learning, data augmentation, surrogate model*

In the manufacturing industry, it is important to produce better products within a certain period for shortening of product lifecycles. Since a large number of computational simulation cases are required in the initial study stage of development. In order to shorten evaluation period, machine learning technologies and 1D-CAE becomes popular in addition to conventional CAE evaluation[1].

The use of predictive models based on deep learning as a substitute for CAE is one of the evaluation methods. While we have much expectations for high accuracy, the applications to engineering problems are not enough to satisfy the expecations[2]. In the fields of material design and computational fluid dynamics, good results have been reported, because huge amounts of data are eventually generated in those research fields[3]. Therefore, the objective of this study is a construction of framework using machine learning technology to evaluate crash box corruption for a significant reduction of CAE analysis cost.

The structural strength evaluation of crash boxes is predicted by machine learning in this study. The training data was obtained from the dynamic elastic plastic analysis of the crash box. The input physical quantities are barrier angle, box thickness, material properties and mass equivalent to vehicle weight. The output physical quantity is the reaction force. F-S diagram is predicted by deep learning using convolutional neural networks with data augmentation for regression problem. Buckling is occurring in the analysis and different directions of curruptions are one of the most interesting phenomenon from a point of engineering view.

We have several difficulties to construct the surrogate model, because of imbalanced frequency problem and The time series of the reaction force maxima is different depending on the data. W'd like to propose an adaptive method for machine learning in structural evaluation that can be used for a wide range of structural evaluations.

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Data augmentation technique for construction engineering regression surrogate model

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Key Words: *Surrogate model, data augmentation, convolutional neural network, deep learning,*

In these days there is a trend to utilize simulation-based verification more frequently rather than verification through experiments using the product in the field of industrial product design. In this context, a development of an evaluation method instead of CAE is needed for more effective designing of industrial products. Machine learning methodology is one of the most anticipated way to accelerate evaluation process.

An application of a surrogate model in deep learning to engineering problems is still studied. In the our researches [1][2][3] the surrogate model using machine learning can predict physical phenomenon within 7% error compared with CAE prediction. The accuracy of the prediction is improved by augmentation technique, which is called as oversampling to avoid overfitting. The augmentation is conducted using data sets with low prediction accuracy.

The objective of this research is studying effective data augmentation for engineering regression problem. SMOTE is based on classification algorithm, however an engineering interpolation should be computed based on physical meanings and influential parameters.

In the machine learning the pedestrian kinematic response with a front part of a car is predicted and the predictor evaluates pedestrian's damage. The responses which are used as learning data are generated by 1D-CAE system. The prediction of the response can be achieved with less than 7% average error using all of data sets. Numbers of training data sets are varied in order to show the enough number and the predictor is evaluated for its accuracy. We'd like to discuss necessary of total number of training data sets and effectiveness of data augmentation.

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Defects Analysis in Carbon Fiber Reinforced Plastic by Combining Machine Learning and Infrared Stress Analysis

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Key Words: *Machine Learning, Defect Analysis, Finite Element Method, Infrared Stress Analysis, Carbon-Fiber-Reinforced Plastic*

The degradation of Carbon Fiber Reinforced Plastic (CFRP) occurs due to damages such as delamination, fiber breakage and matrix crack. Therefore, we need to conduct high-precision and efficient Non-destructive testing (NDT). Examples of NDT are ultrasonic examination, X-ray tomography and infrared analysis. In ultrasonic examination, objects are required in the water. In X-ray tomography, we need to set object in an analysing room. Hence it is suitable to analyze large structures by means of infrared analysis. In addition, it is hard to estimate the three-dimensional information of defects by means of most of these NDT methods. To solve these problems, some studies propose machine-learning-aided NDT. In this study, we developed an inverse analysis model that predicts the spatial information of defects from the distribution of sum of the principal stress on the surface (DSPSS). The DSPSS is calculated from the temperature change measured by infrared analysis in both experiments and numerical analysis. This inverse analysis model is proposed as an alternative method to the existing damage analysis. Inverse analysis model is composed of two machine learning models. One is for making experimental DSPSS closer to the results of the Finite Element Method (FEM) and the other is for predicting the spatial information of defects from DSPSS by FEM analysis. The proof of concept has been successfully done for the model which predicts the spatial information of defects from FEM analysis [1]. We use U-net [2] for the first machine learning model and Convolutional Neural Network (CNN) for the second one.

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Finite element quantitative analysis and deep learning qualitative estimation in structural engineering

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Key Words: *Finite element, quantitative analysis, deep learning, structural engineering*

Finite element method (FEM) has been widely used to study the mechanics of materials and solids, as well as fluid–structure interactions, and building construction strategies. FEM is popular all over the world with the development of computer technology. It is known for powerful computing ability, surpassing humans in computing. In this context, in addition to teaching engineers to use FEM calculation software, structural engineering education in the past nearly two decades also focuses on cultivating engineers' ability of qualitative analysis. However, the rapid development of deep learning methods in recent years means that human qualitative analysis capabilities based on rules of thumb will also be replaced by artificial intelligence. The main question of this study is: what role will deep learning methods play in the future structural analysis? In this paper, a large number of finite element analyses are carried out for three classic boundary value problems, such as the behaviour of wires under load, the problem of heat conduction, and plane strain. The deep learning model is trained with FEM simulation results. It can quickly and accurately predict the results of related similar problems, and evaluate the accuracy and efficiency. The results show that artificial intelligence can to some extent replace the work of human qualitative analysis based on rules of thumb. Predictions and expectations about the role of deep learning methods in future structural analysis processes are given.

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Generating Merging Strategies for Connected Autonomous Vehicles Based on Collaborative Spatiotemporal Information Sensing and Multi-agent Deep Reinforcement Learning

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Key Words: *Mixed traffic flow; multi-agent deep reinforcement learning; cooperative control; spatiotemporal information fusion*

A major challenging issue concerning the mixed traffic flow, composed of connected autonomous vehicles (CAV) and human driving vehicles (HDV), is how to improve overall efficiency and safety by assigning collaborate control strategies to CAVs. Multi-agent deep reinforcement learning (MADRL) is a promising approach to address the challenge [1]. It enables the joint training of multiple CAVs by using CAV sensing information and does not need the compliance of HDVs. However, the design of collaborative sensing is non-trivial, especially when there are dynamic numbers of HDVs surrounding a CAV and dynamic numbers of CAVs in the mixed traffic flow system. Under such conditions, the conventional MADRL with fixed neural network structures is no longer effective [2]. In this regard, this paper designs a hierarchical spatiotemporal information extraction module and uses a multi-agent deep Q network (MADQN) to output safe and collaborative lane change decisions of CAVs. More specifically, within the local perception range of every CAV, a long-short term memory neural network with attention mechanism (A-LSTMNN) is employed to extract the sequential motion information and to anticipate the behavior of surrounding HDVs. Then the anticipated and current motion information collected and extracted by each single CAV is aggregated by a graph convolution network (GCN), to realize a collaborative sensing of multiple CAVs. We then propose a hybrid control framework incorporating the spatiotemporal information extraction module into the MADQN, termed as spatiotemporal deep Q network (STDQN), to generate merging strategies for multiple CAVs. The simulation experiment is conducted in an onramp merging scenario, which is one of the most important and commonly seen scenarios in a highway system. Experiment results prove that by using our proposed control framework, the overall traffic efficiency and safety can be improved as compared to baseline MADRL and rule-based methods. The proposed framework can be deployed into a real traffic environment to realize proactive traffic management.

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Graph and Machine Learning-based Approach to Prediction of Ultimate Load of Latticed Shells Considering Geometric Nonlinearity

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Key Words: *Machine learning, Supervised learning, Graph embedding, Non-linear buckling load, Truss, Shell*

Latticed shells are structures that represent curved surface shapes using beam or bar elements and are widely adopted to cover large spaces. Considering the cost and environmental performance, latticed shells need to be designed with slenderer members as much as possible, but the risk of buckling and yielding increases at the same time. Therefore, it is important to design structural shapes and member sizes considering this dilemma in a balanced manner.

Linear buckling loads often overestimate the value computed by the buckling analysis considering geometric nonlinearity. For this reason, geometrically nonlinear buckling analysis is more accurate to measure structural stability. Furthermore, stress analysis considering geometric nonlinearity is preferable for thin-shell structures because small deflection induces large variation in the equilibrium state. However, geometrically nonlinear analysis requires computationally expensive analysis to trace the equilibrium path.

If an approximate model that can estimate the ultimate load at a small computational cost can be introduced, it will be possible to consider the geometric nonlinearity from the early stage of structural design without worrying about the computational cost. Zhu et al. [1] introduced artificial neural networks and support vector regression, which are standard machine learning (ML) models, to predict the reduction ratio of the nonlinear buckling load of reticulated shells at a low computational cost.

This study develops a prediction model for the nonlinear buckling load of latticed shells by combining graph embedding (GE) and machine learning (ML). A graph is a data structure consisting of vertices and edges, and the structural information of latticed shells is expressed in the form of graphs. GE is a method of extracting features by considering the connectivity of graphs [2]. By combining this method with supervised learning, which is a class of the ML methods, the ML model is trained to estimate nonlinear buckling loads for various latticed shells.

This method can be used to train models for small-scale latticed shells, and the trained models can be applied to larger-scale ones without training. The computational cost required for training and the prediction accuracy of the trained model are verified through numerical examples and reported in the presentation.

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Physics-Informed Neural Networks for Prediction of Ground Settlement

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Key Words: *PINN, Deep learning, Neural network, Consolidation settlement*

The long-term consolidation settlement, which is one of significant considerations in the constructions of port facilities, is often evaluated by the numerical analysis. However, it requires high computational resources to construct and calculate the numerical models that are on the physics validities. In this study, the applicability and effectiveness of the Physics-informed Neural Network (PINN) to the calculation of long-term consolidation settlements are verified for the aims of its accurate evaluations with low computational costs. The PINN is one of deep learning models considering the physics law represented by the partial differential equation (PDE) in the loss function, that was proposed by Raissi et al. [1]. It can solve the black-box problem in the use of neural network since the consideration of PDE is clearly assured. A simple model of a single clay layer was considered in this study for the verification of PINN performance. The Mikasa's consolidation equation shown below was adopted as the governing equation to predict the strain due to the consolidation.

$$\frac{\partial \varepsilon_{(z,t)}}{\partial t} = C_v \frac{\partial^2 \varepsilon_{(z,t)}}{\partial z^2} \tag{1}$$

where ε, z, t, Cv, are strain, depth of ground, time from the start of loading, and consolidation coefficient, respectively. The strain values at random times and depths of 10 days after the start of loading, created by solving the PDE and adding 10% noise, were used for the training data. In the constructed PINN model, the predicted strain distribution after 100 days was more accurate than that in the NN, that was constructed without physics knowledge for comparison, even for training data with the noise. Additionally, the constructed PINN was shown to provide the prediction of long-term consolidation settlement at any timing with good agreements to exact data. From these results, the improvement of prediction accuracies and also the effectiveness of PINN to the inverse analysis of soil parameters, such as consolidation coefficient, are expected.

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Physics-informed neural networks for structural shell elements

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Key Words: Physics-informed Neural Networks, Shell Structures, Finite Element Method, Ill-Posed Problems

Shell structures are ubiquitous structural elements found both in nature and society. As the out-of-plane dimension of such structures is much smaller than the in-plane dimensions, one can employ a reduced two-dimensional formulation to simplify their mechanical description. While such theories are mathematically elegant and have shown to be good approximations for small thicknesses, their numerical implementation by means of the finite element (FE) method is notoriously challenging. This is mainly due to the technical formulation rooted in differential geometry and numerical challenges such as shear and membrane locking arising, e.g., for pure bending deformations in the thin-thickness limit, due to limitations of the chosen function space.

While a variety of techniques have been proposed to bypass such limitations in the FE setting, we investigate the use of Physics-informed Neural Networks (PINNs), which can be understood as highly nonlinear function approximators, to solve the Naghdi shell equations in both their strong and weak form. We present encouraging numerical studies that demonstrate the capability of PINNs to accurately approximate the results obtained via FE for a variety of different shell geometries.

Furthermore, PINNs appear to be able to overcome the classical locking observed in FE, although the convergence to the numerical solution worsens in the thin-thickness limit due to an increasingly ill-posed loss function and stiff gradient flow. We expand this discussion and highlight why current techniques in the literature fail to mitigate such problems.

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Prediction of physical property of fiber-reinforce composite materials using deep neural network

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Key Words: *Deep Learning, Neural Network, Surrogate Model, Fiber Reinforce composite materials*

In the field of numerical simulations, a data-driven approach called surrogate model, in which some or all of numerical calculations are replaced by machine learning, is attracting attention. Models using deep neural networks have the potential to replace complex numerical calculations. It is proposed to be used in a wide range of numerical calculations such as structural analysis[1], fluid analysis[2], process simulations[3] and so on.

However, a large-scale deep neural network that can replace complicated numerical calculations requires a large amount of data for learning because the number of parameters is enormous. On the other hand, many numerical calculations require enormous calculation time and resources, and it is often difficult to generate a large amount of learning data. Therefore, a surrogate model needs to be constructed a highly accurate model with a small amount of data.

In this study, a surrogate model that predicts the physical properties of representative volume elements of fiber-reinforced composites with a knitted structure is constructed. We investigated a method for constructing a prediction model with the same accuracy as when using a large amount of data even with a small amount of data. It was confirmed that it is possible to improve the accuracy by appropriately expanding the data even with a small amount of data. We'd like to discuss how much accurate prediction is achieved and the effectiveness of the model in the design process.

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Prediction of warp distortion in circuit board using machine learning

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Key Words: *Machine Learning, Deep Learning, Data Augmentation, Regression Prediction*

Lead-free solder has become common as environmental concerns increase. Since the maximum temperature of furnace has been increased by the solder, the temperature conditions has become strict. Defects of solder joint have increased due to circuit board warp. If the displacement of board warp is predicted, the defects will be decreased by modification of product design. In this study, we'd like to employ a convolutional neural network, characterize the data relations as a feature, for the prediction of circuit board warpage. The objective is a prediction of the amount of board warp using very limited results of several experimental measurements.

All of input data which include material properties and so on are standardized between 0 to 1. The output data is standardized warp displacement of 9 points in vertical direction on the surface of circuit board. Since a number of original data is very limited, it is necessary to augment training data sets. However, usual augmentation techniques just interpolate closed data in a parameter space. In short, the improvement of the prediction accuracy is limited. We'd like to propose a method called as factor levels augmentation. The fundamental factor levels augmentation is linear interpolation, however it may not be able to represent actual physical phenomena which usually contains nonlinearity. Nonlinear interpolation according to physical phenomenon produces better training data sets.

Prediction accuracies between no augmentation data and factor levels data augmentation is compared. In the case of no augmentation, the prediction results include 40 errors over 20%. In the case of factor levels augmentation, the highest errors are less than 5%. The significance of the factor levels augmentation is confirmed. It is important to keep the trend and characteristics of the dataset remember when using factor levels augmentation so that points with different trends are not taken. We'd like to discuss more appropriate general data augmentation techniques using a smaller number of original data.

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Bayesian Inversion of a Coupled Acoustic–Gravity Model for Predictive Tsunami Simulation

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Key Words: Bayesian Inversion, Tsunami Modeling, Inverse Acoustics, Surrogate Operators

To improve tsunami preparedness, early-alert systems and real-time monitoring are essential. We propose a novel approach for predictive tsunami modeling within the Bayesian inversion framework. This effort focuses on informing the immediate response to an occurring tsunami event using near-field data observation. Our forward model is based on a coupled acoustic–gravity model (e.g., [1]). Similar to other tsunami models, our forward model relies on transient boundary data describing the location and magnitude of the seafloor deformation. In a real-time scenario, these parameter fields must be inferred from a variety of measurements, including observations from pressure gauges mounted on the seafloor. One particular difficulty of this inference problem lies in the accurate inversion from sparse pressure data recorded in the near-field where strong hydroacoustic waves propagate in the compressible ocean; these acoustic waves complicate the task of estimating the hydrostatic pressure changes related to the forming surface gravity wave. Furthermore, the forward model incurs a high computational complexity, since the pressure waves must be resolved in the 3D compressible ocean over a sufficiently long time span. Due to the infeasibility of rapidly solving the corresponding inverse problem for the fully discretized space-time operator, we explore options for using surrogate operators of the parameter-to-observable map.

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Learning High Dimensional Parametric Maps from Limited Training Data

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Key Words:

Outer-loop problems arising in engineering applications (such as optimization, uncertainty quantification and inverse problems) require repeated evaluation of computationally intensive numerical models, such as those arising from discretization and solution of ordinary and partial differential equations, for many different choices of model parameters. The cost of these evaluations makes solution using the model prohibitive, and efficient accurate surrogates are a key to solving these high dimensional problems in practice. In this talk we will discuss various projected neural network strategies that bypass the high fidelity parametric mapping by learning informed modes of the mapping. These neural networks can be used in place of a high fidelity model to enable the solution of high dimensional outer-loop problems. These strategies include reduced basis projections, adaptive construction of residual neural networks and compression of derivative information that can be used both to construct and train neural networks. These reduced-basis architectural strategies outperform conventional data-driven approaches when limited training data are available due to computational costs of evaluating high dimensional nonlinear PDEs.

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Multi-fidelity Hamiltonian Monte Carlo with Deep Learning-based Surrogate

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Key Words: Hamiltonian Monte Carlo (HMC), Bayesian inversion, Scientific machine learning (SciML), Multi-fidelity modeling, Uncertainty quantification (UQ)

In recent years, Hamiltonian Monte Carlo (HMC) method has emerged as a state-of-the-art Markov chain Monte Carlo (MCMC) technique that exploits the geometry of the target distribution to generate samples in high dimensional space in an efficient manner. Despite its impressive empirical success and increasing popularity, its wide-scale adoption (in PDE-based models) is still limited due to the high computational cost associated with the gradient calculation at every step. Furthermore, application of this method is simply not possible in scenarios where the gradient of the posterior cannot be computed (for example, with black-box simulators and/or with non-differentiable priors). To overcome these challenges, we propose a novel multi-fidelity Hamiltonian Monte Carlo algorithm. In this two-stage algorithm the acceptance probability is computed in the first stage via standard HMC proposal using an inexpensive surrogate model (with easy-to-compute-gradients), and, if the proposal is accepted, the full posterior is evaluated using the high fidelity (HF) numerical solver in the second stage. Splitting the standard HMC algorithm into these two stages allows for the efficient and computationally inexpensive evaluation of the gradient of the posterior (by leveraging automatic differentiation capabilities of DL-based forward model surrogate for example), thus retaining advantages of HMC, such as scalability to high dimensions and faster convergence while producing accurate posterior samples by using HF numerical solvers in the second stage in forward mode. We demonstrate the effectiveness of the proposed algorithm on a variety of linear and non-linear Bayesian inverse problems using traditional and modern deep generative priors [1] and showcase that in all scenarios it significantly outperforms the traditional HMC algorithm in computational efficiency while retaining similar accuracy.

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Operator Learning for Forward and Inverse Problems

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Key Words: Operator Learning, UQ, Convergence Rate, Bayesian Inference, Parametric PDE, Surrogate

Operator learning has emerged as a key enabler for accelerating the computation of existing scientific models [1] and for discovering new models from data when no model exists [3]. In this talk, I will describe recent scientific machine learning methodologies that are designed to scalably and efficiently emulate (potentially noisy and nonlinear) operators that define forward and inverse problems arising in science and engineering. Crucially, these methods are conceptualized on infinite-dimensional input and output function spaces and thus can handle parameters of arbitrarily high dimension after discretization.

The first contribution is a hierarchical operator regression approach [2] that generalizes traditional random feature methods operating between Euclidean spaces. Viewed as a randomized kernel method with a data-adapted feature map, it enjoys several computational advantages over its nonparametric counterparts, and through its Gaussian process connection, is naturally interpretable and provides automatic uncertainty quantification. The algorithm is used to regress parametric solution maps defined by nonlinear partial differential equations (PDEs) and rapidly solve PDE-based Bayesian inverse problems.

Moving on to theoretical advances, in the setting of learning linear operators I will provide large data convergence rates of nonparametric statistical estimators that give sharp in-distribution and out-of-distribution generalization guarantees in infinite dimensions [4]. The theory is valid not only for bounded or compact operators, but also for unbounded ones; a key conclusion of relevance to data-driven model discovery is that unbounded linear operators such as those appearing in linear PDEs require more training data to achieve a fixed error tolerance than do compact operators. Finally, I will remark on methods that directly learn the observation-to-parameter solution operator of linear and nonlinear ill-posed inverse problems.

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Deep Learning-driven Real-time Concurrent Multi-Scale Topology Design Optimization of Fiber-reinforced Composite Laminates

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Key Words: *Concurrent Multi-scale Design Optimization; Deep Learning-Driven Topology Design Optimization; Real-time Topology Optimization; Discrete Material Optimization; Additive Manufacturing Constraints*

Abstract The multi-scale design optimization of fiber-reinforced composite laminates has shown great potential in structural lightweight and functionalization and has become a research hotspot in recent years, especially with the development of composite additive manufacturing technology. Compared with traditional isotropic material structural topology optimization, concurrent multi-scale variable stiffness design optimization of composite laminates poses a greater challenge for large-scale design variables, constraint calculations, and real-time topology optimization. Based on these, the present paper investigates the concurrent multi-scale variable stiffness design optimization of fiber-reinforced composite laminates based on deep learning. Based on the convolutional neural network (CNN) method, a new deep learning approximate model for real-time concurrent multi-scale variable stiffness design optimization of fiber-reinforced composite laminates is proposed. In the proposed model, the initial element artificial density, discrete fiber laying angels, optimized macroscopic topology configuration, and optimized microscopic fiber laying angels are inputted as samples under random loading conditions for the deep learning CNN training. The optimization of 2D composite panels demonstrates the capabilities of the proposed framework. Numerical studies show that the proposed deep learning-driven model can realize real-time concurrent multi-scale variable stiffness design optimization of fiber-reinforced composite laminates, which provides a real-time choice for the design of composite structures in engineering applications.

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Optimization of turbine airfoil using deep reinforcement learning

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Key Words: *Deep Reinforcement learning, Turbine Optimization,*

Turbine design requires intensive human labour costs because expert designers have to modify shape parameters manually. It is desired to optimize turbine design parameters, but the flow around the turbine is complicated and difficult to optimize using conventional optimization methods. In addition, designers have to optimize intensive number of airfoils whose flow conditions are slightly different from each other. If conventional optimization methods are employed, we have to solve different optimization problem for each design condition, which is inefficient and is not acceptable from practical point of view. In the present study, the reinforcement learning based optimization method is proposed that can handle such flow characteristics. The proposed method needs to be trained using intensive training dataset, but once it is trained, the trained model is reusable for different flow conditions; the proposed method can optimize turbine airfoils in a small time period.

Reinforcement learning is one of a unsupervised learning methods, which was successfully applied to optimal control and arcade games. Recently, reinforcement learning was also applied to mechanical and structural design optimization [1,2]. In the present study, RL model is trained to inputs information including flow field information and outputs optimal way to modify airfoil shape. The capability of dealing with unseen tasks, i.e. capability to optimize airfoil in different flow condition, is examined using numerical experiments.

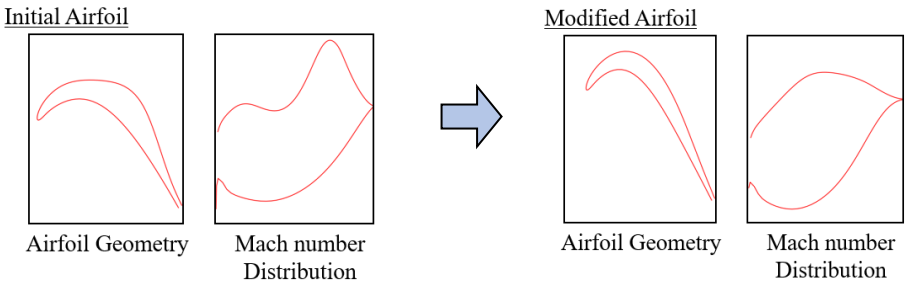

Fig. 1 Example of initial airfoil and optimized airfoil by the proposed method

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Real-Time Structure Topology Optimization using CNN driven Moving Morphable Component Method

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Key Words: *MMC, Topology Optimization, Real-Time Optimization, Convolutional Neural Network, Deep Learning*

Based on the moving morphable component (MMC) method, a real-time Topology Optimization (TO) algorithm using a convolutional neural network (CNN) is presented. Comparing to the Solid Isotropic Material with Penalization (SIMP) TO method, MMC method describes the optimization structure together with level set function, which causes difficulty and complexity in using deep learning model with MMC method. In this study, a new data preprocessing method is proposed to ensure that the CNN model can be trained based on the accuracy structure boundary information. Meanwhile, such method can also help the CNN model capture data features with limited sample set. To avoid the component dislocation, the topology optimization boundary information of the optimized results is used as the sample set label. The new algorithm was implemented with several examples, the efficiency and effectiveness have been verified. The trained deep learning model can significantly improve the optimization efficiency of MMC method and offer accurate results with clear boundary. This study provides a new theoretical basis and numerical algorithm for real-time topology optimization of structures.

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Real-time Topology Optimization Design of Heat Dissipation Structure Based on CNN Framework

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Key Words: *Real-time Topology Optimization, Convolutional Neural Network, Neural Network, Heat Dissipation Structure, MMC Topology Optimization Framework*

In the present study, a real-time topology optimization framework of heat dissipation structure is established by combining Convolutional Neural Network (CNN) model with the Moving Morphable Components (MMC) framework. The optimized topology is obtained in real-time while ensuring more efficient heat dissipation performance of the structure. This is because the clear geometric profile of the optimized topology structure can be directly obtained without any results post-processing work based on the MMC framework. The present study innovatively proposes a data pre-processing method for the MMC framework, so that it can be trained based on a small sample set to obtain sufficiently high-precision prediction results. At the same time, the optimized topology configuration is used as the training label of the model, which avoids the secondary processing of graph generation and reduces the data error. Numerical examples show the topological configuration of the structure under different heat sources and boundary conditions, which shows the effectiveness and superiority of the framework.

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Topological Design of Grid Stiffened Structures

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Key Words: *Topology optimization, Stiffened Structures, Deep learning*

Grid stiffened structures generally achieve various excellent properties through geometry and topology design of the stiffeners. However, it is difficult to obtain the optimal result only by empirical design, and it is impractical to explore the design space through repeated experiments. Topology optimization is one of promising methods applied to the design optimization of structures with multiscale characteristics. In the design optimization of grid stiffened structures, the optimum layout and types of the stiffeners should be solved. However, due to the high-dimensional topological design space, multiple local optima, and high computational cost, there still exist some challenges in realizing accurate inverse design. To address these obstacles, we will propose the design framework based on the gradient based optimization algorithm with the help of the deep learning, where a microstructure database will be established and discussed. The optimization formulation of reinforced ribs of thin-walled stiffened structures for minimizing the vibration response and maximizing buckling load is established. The optimum layout of stiffeners is realized in several numerical examples of stiffened plates to verify the effectiveness of the proposed method.

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A data-driven, physics-compatible approach to model history-dependent materials

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Key Words: Data-driven, Computational mechanics, History-dependent materials, Internal variables, Interpolation

In this work, a general view of data-driven computational solid mechanics, suitable for history-dependent materials, is developed within the Thermodynamics of Irreversible Processes framework. It is based on the Experimental Constitutive Manifold (ECM) concept. The mathematical structure of the ECM, which involves internal state variables, constitutes the material model associated with the available experimental data. The hidden variables are not known a priori but are calculated from the experimental data thanks to the so-called "ECM-Central Problem". A second and equally important step is defining the mathematical model as an interpolation of the experimental data obtained from the various tests carried out. That leads to a model very similar (mathematically speaking) to the standard models encountered in Materials Science. We use a kernel-based interpolation associated with a Reproducing Kernel Hilbert Space, which is very efficient here because the functions involved are very regular.

This paper presents recent advances in this data-driven computational approach, particularly the interpolation procedure used. Illustrations are given on the modeling of elasto-plasticity, for which we propose data-driven models for isotropic materials in which no a priori assumptions on the modeling are necessary.

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A Mechanics-Informed Artificial Neural Network Approach in Data-Driven Constitutive Modeling of Elastic and Viscoelastic Materials

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Key Words: *artificial neural networks, constitutive modeling, elasticity, regression, viscoelasticity*

A mechanics-informed, data-driven framework for learning the constitutive law of a complex material from stress-strain data is proposed. It features a robust and accurate method for training a regression-based, surrogate model capable of capturing highly nonlinear material behavior while preserving principles that are important to solid mechanics. In this sense, the proposed modelling framework is structure-preserving. The model it generates combines the form-agnostic advantage of purely phenomenological data-driven regressions and the physical soundness of mechanistic models. The underlying training procedure is equally compatible with both numerical and experimental stress-strain data.

While regression Artificial Neural Networks (ANNs) have excellent nonlinear function fitting capabilities, an ANN-based constitutive law that fits well to training data is not necessarily physically sound or exploitable in the context of a numerical simulation, due to imperfect training convergence, noise in the data, overfitting, and most importantly, the absence of mechanics (or physics)-based constraints. Therefore, the proposed framework supplements a typical ANN loss function with mechanics-informed contributions and enforces desirable mathematical properties on the network architecture, to guarantee the satisfaction of important physical properties regardless of training accuracy or training data quality. Furthermore, by embedding *a priori* a knowledge of mechanics into the model it constructs, the proposed framework favors the learning of the structure of a constitutive relation rather than overfitting to the training data. As such, it also regularizes the model it generates, reduces its sensitivity to training data noise, and promotes its robustness to inputs outside of the training domain.

First, the proposed framework is presented in the nonlinear elastic setting, as in [1], where the stress depends only on the instantaneous strain state. Various physics-based model constraints important for elasticity are discussed and formulated in the context of an ANN, including dynamic stability, material stability, objectivity, and preservation of rigid body modes. Next, the framework is extended to the viscoelastic setting, where the stress depends on both the strain and strain-rate, using two-different approaches that are informed by thermodynamic constraints such as the Clausius-Duhem inequality.

Finally, the performance of the proposed framework for data-driven modelling is illustrated with the nonlinear, dynamic, multiscale simulation of the supersonic inflation of an atmospheric aerodynamic decelerator system including a parachute canopy made of a woven fabric. It is shown to enable the computational tractability of the chosen homogenization approach and to reproduce flight test data.

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A PDE-Based Transformation Method for Model Order Reduction of Nonlinear Geometrically Parameterized Microstructures

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Key Words: *Reduced Order Modelling, Geometrical Transformation, Computational Homogenization, POD, Gaussian Process Regression, Shape Optimization*

With the recent advances in additive manufacturing and in the field of metamaterials, designing microstructures has become a topic of high interest. To better understand structure-property relations for such microstructures, computational homogenization is typically used. The microstructure is explicitly modelled on a representative volume element, and thus replaces the macroscopic constitutive model with an effective one. Such procedure becomes computationally expensive and typically infeasible in the context of uncertainty quantification, material design and optimization, where numerous simulations must be run.

To make these analyses amenable, the parameterized microscopic problem is often approximated with an inexpensive-to-evaluate surrogate model, using for example data-driven methods from Machine Learning and Deep Learning. For optimization or inverse problems, the surrogate model must be able to handle different types of parameters (e.g., loading, material and geometry). In a recent work [1], we successfully constructed an accurate surrogate model for microstructures under varying loading and material parameters by approximating the microscopic stress field with proper orthogonal decomposition (POD) and finding the coefficients with Gaussian process regression (GPR).

In this work, we extend our previous methodology to also treat geometrical parameters. The main hurdle for geometrically parameterized problems lies in finding geometrical transformations that map each snapshot onto a common reference domain. After finding such a transformation, the same procedure as before (POD and GPR) can be adopted. Most existing works describe these transformations using free form deformations or radial basis functions (see, e.g., [2]). Instead, we obtain the transformation map by solving an auxiliary linear partial differential equation (see, e.g., [3]) and show how this, combined with the nonlinear microscopic problem, can be used to learn an accurate and fast-to-evaluate effective constitutive model. Moreover, we show that the predicted stress fields automatically fulfil the microscopic physics (balance laws and periodicity) for any parameter values.

The proposed method is tested on several composite microstructures, involving rotations and large variations in shape of considered inclusions. The examples involve two scales, showcasing a high accuracy and speedup, and its potential in two-scale shape optimization and material design.

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A Physics-informed Complementary Energy Form in Solid Mechanics

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Key Words: Physics-informed neural network, Deep energy method, Deep neural network

Many physical phenomena are modeled by partial differential equations (PDEs). In general, it is difficult to obtain the analytical solutions of PDEs. Hence, various numerical methods are developed to obtain the approximate solutions in a finite-dimensional space. Traditional ways to tackle the solution of PDEs are the finite element method, the finite difference method, the finite volume method, and mesh-free method. In the present day, deep learning is ubiquitous, empowering various fields. The success of deep learning is partially attributed to the powerful approximation capabilities of the neural network. It is natural to use the neural network as the approximation function of PDEs, i.e., physics-informed neural network (PINN). Another framework of PINN is the deep energy form (DEM), using the physical potential energy as the optimized loss function. Although DEM has the minimum potential energy formulation, the DEM lacks the principle of minimum complementary energy formulation. In this study, we propose the complementary energy form of DEM. We compare the PINN strong form and different energy forms including minimum potential and minimum complementary form. The accuracy and efficiency are carefully examined by applying different PINN methods to three loading cases of solid mechanics benchmark: only Dirichlet boundary condition, only Neumann boundary condition, and mixed boundary condition. Through the comparison with the analytical solution, it is found that: (1) DEM of minimum complementary energy form is suitable for handling the case of only Dirichlet boundary condition, (2) DEM of minimum potential energy form is suitable for handling the case of only Neumann boundary condition. Compared with PINN strong form, DEM shows certain advantages in terms of the simplicity of hyperparameter tuning and the computational efficiency due to the high tensor field in solid mechanics.

Adaptive Goal-oriented Phase Space Sampling in Data-Driven Computational Mechanics

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Key Words: *Data-Driven Computing, Inelastic Material Behavior, Efficiency of Data-Driven Solvers*

The Data-Driven (DD) computing paradigm in mechanics problems [1] aims to obviate the need for empirical constitutive modeling, by directly using data from physical experiments and lower-scale computations to capture material behavior, while retaining all essential constraints and conservation laws. The goal of the data-driven solver is to determine, for every material point of a discretized system, the optimal local state, i.e. the material state (stress, strain) which results in the closest possible satisfaction of compatibility and equilibrium, by searching within the data set. The question of how to efficiently generate a data set suited for a particular application (i.e. goal-oriented) is still an open problem, particularly in the case of history-dependent material behavior.

The objective of this study is to develop an unsupervised goal-oriented data sampling algorithm furnishing an efficient DD scheme that converges in global distance. The idea is to iteratively expand an initial data set until this distance is acceptably small. We first analyze the spatial distribution of stress-strain paths in the material points and their corresponding distances from the data set. This analysis is used to propose new paths to be sampled using lower scale RVE calculations, and added to the preexisting data set. This process is repeated until the local state of each material point is well covered by the expanded data set.

To demonstrate the method, we carry out DD finite element simulations of a specimen of Hostun sand, a material with complex history-dependent behavior, subjected to triaxial compression [2, 3]. The sampling of the phase space of the local strain-stress pairs is performed with LS-DEM calculations of representative unit cells, subjected to loading paths determined by the proposed sampling algorithm, while material history is accounted for through a thermodynamically-motivated parameterization of the data sets [2]. It is shown that this adaptive expansion of the data set, tailored for the particular application, leads to superior convergence properties compared to preexisting sampling techniques, which can facilitate further applications of the DD computing paradigm.

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Bayesian Neural Networks for Weak Solution of PDEs with Uncertainty Quantification

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Key Words: Weak Form, Bayesian Neural Network, Uncertainty Quantification, Nonlinear Elasticity, PDE Solver, Partial Differential Equations

We will present our recent advance in Bayesian neural networks for weak solution of partial differential equations (PDEs) with uncertainty quantification [1]. Solving PDEs is the canonical approach for understanding the behavior of physical systems. However, large scale solutions of PDEs using state of the art discretization techniques remains an expensive proposition. In this work, a new physics-constrained neural network (NN) approach is proposed to solve PDEs without labels, with a view to enabling high-throughput solutions in support of design and decision-making. Distinct from existing physics-informed NN approaches, where the strong form or weak form of PDEs are used to construct the loss function, we write the loss function of NNs based on the discretized residual of PDEs through an efficient, convolutional operator-based, and vectorized implementation. We explore an encoder-decoder NN structure for both deterministic and probabilistic models, with Bayesian NNs (BNNs) for the latter, which allow us to quantify both epistemic uncertainty from model parameters and aleatoric uncertainty from noise in the data. For BNNs, the discretized residual is used to construct the likelihood function. In our approach, both deterministic and probabilistic convolutional layers are used to learn the applied boundary conditions (BCs) and to detect the problem domain. As both Dirichlet and Neumann BCs are specified as inputs to NNs, a single NN can solve for similar physics, but with different BCs and on a number of problem domains. The trained surrogate PDE solvers can also make interpolating and extrapolating (to a certain extent) predictions for BCs that they were not exposed to during training. Such surrogate models are of particular importance for problems, where similar types of PDEs need to be repeatedly solved for many times with slight variations. We demonstrate the capability and performance of the proposed framework by applying it to different steady-state and equilibrium boundary value problems with physics that spans diffusion, linear elasticity, and nonlinear elasticity.

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Constitutive Modeling of Isotropic and Anisotropic Hyperelastic Materials based on Physically Constrained Artificial Neural Networks

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Key Words: Data-based modeling, Artificial neural networks, Hyperelasticity, Multiscale approach

The formulation and calibration of constitutive models is still a challenging task for materials which reveal complex nonlinear behavior. Due to this, numerous novel approaches – generally referred to as data-based methods – have recently arisen in the computational mechanics community [1]. In this contribution, an automated artificial neural network (ANN)-based strategy for the efficient description of isotropic and anisotropic hyperelastic solids is presented. Starting from a large data set comprising deformation and corresponding stresses, a physically based transformation of the problem into the space of invariants is performed. It enables to reduce the cardinality of the data set by several orders of magnitude. The thinned data set is then used to calibrate physically informed ANNs as a constitutive model within a customized training process. Thereby, the set of invariants serves as the input instead of the deformation tensor itself which automatically introduces material symmetry [2]. Furthermore, in order to fulfill the 2nd law of thermodynamics, the ANN is utilized on the energy level.

The proposed method is exemplarily shown for the description of highly nonlinear elastic materials in several demonstrative examples [2]. Thereby, the necessary data sets are generated synthetically, i. e., they are collected from virtual experiments of samples comprising a constitutive behavior defined by classical nonlinear models. It is shown that the trained ANN is able to achieve a high accuracy within fully three-dimensional simulations, although the training data are taken from pure two-dimensional plane stress states. Furthermore, the method is applied within a data-based multiscale approach, where the ANN serves as a surrogate or macroscopic model describing the effective behavior of periodic unit cells. To train the network, a data set is generated via offline computational homogenizations. The specific microstructural geometry of the considered unit cells is included within the macroscopic ANN-model via a related set of invariants. Consequently, the presented approach enables the solution of multiscale problems with comparatively low computational cost.

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Data-driven Constitutive Laws for Hyperelasticity in Principal Space: Numerical Challenges and Remedies

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Key Words: Data-Driven Constitutive Relations, Artificial neural network, Hyperelasticity

Artificial neural networks (ANNs) have been employed to represent the constitutive relation of hyperelastic materials under large deformations. Various advancements have been made in order to obtain improved model performance, e.g. by incorporating certain physical constrains [1, 2]. However, most of these approaches still suffer from numerical instability during the numerical solution procedure. This contribution discusses a formalism for data-driven modelling of advanced materials with special interest in the large deformation response of three-dimensional specimens. The underlying hyperelastic deformation problem is formulated in the principal space using principal stretches and principal stresses. The associated constitutive relation is consequently using principal quantities and captured by the parameter-free representation using a deep neural network.

The presentation investigates certain physics-motivated requirements imposed on the architecture of the ANN such as the symmetry of its Jocobian matrix, growth conditions, and objectivity criteria [3]. The training phase of the constitutive ANN operator employs a loss function which ensures the identified consistency conditions. The prediction phase exploits a constitutive blending approach to stabilise the numerical solution procedure in the presence of typically local stretch/stress extrema. The non-convergence effect is overcome by using a modified Newton-Raphson procedure when solving global structural problems using Finite Element Method. The presented approach is implemented using FEniCS [4] and builds on symbolic representation of the ANN operator based on the Unified Form Language (UFL). The neural network is constructed, trained and tested using PyTorch.

Numerical benchmarks demonstrate the ability of the presented complete and general formalism to describe non-trivial load-deformation trajectories of 3D test specimens as well as real-world experiments.

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Data-driven Estimation of Plastic Properties of Alloys with Various Hardening Behaviors Using Neighboring Indentation Test

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Key Words: Elastic-plastic material, finite element method, mechanical testing; response surface, instrumented indentation test, material database

Nowadays, structure materials with high strength, ductility and good strength-to-weight ratio are required for industries. Instrumented indentation test provides an efficient, high through-put and non-destructive way to characterize the mechanical properties of alloys, although it is hard to get the stress-strain relationship corresponding to tensile test directly due to the complex stress state beneath the indenter. Various estimation approaches for the plastic properties have been purposed based on the results of instrumented indentation test [1–3]. In our previous study [4], the interaction effect between two neighboring indentation was utilized to determine the two material constants of a simple constitutive model of plasticity. The purposed approach was validated for application to aluminum alloys and stainless steel, the estimated stress-strain curve agree with the experimental results in aluminum alloys but the linear hardening behavior in stainless steel cannot be followed due to the power-law hardening constitutive model. In this study, a computer-aided approach to estimate the plastic properties of alloys using neighboring indentation test was purposed with a modified constitutive model to represent the various hardening behavior of alloys. The material database to determine a set of material constants for the modified plastic constitutive model was prepared by the finite element simulation of neighboring indentation. The material constants were estimated by load – depth curves and topography of indentation impression from neighboring indentation tests. This approach was validated for application to aluminum alloys and a stainless steel.

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Data-Driven viscoelasticity in the frequency domain

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Key Words: Viscoelasticity, dynamic mechanical analysis (DMA), Data-Driven mechanics, Fourier transform, Wasserstein metric

The classical computational paradigm has been to calibrate empirical material models using observational data and then use the calibrated material models in calculations. This process of modeling, if at all possible, necessarily corrupts the data and adds many uncertainties, especially in complex systems such as biological tissue. Data-Driven computational mechanics is a new paradigm, according to which calculations are carried out directly from empirical material data and pertinent physical constraints such as compatibility and equilibrium, thus bypassing the empirical material modeling step of conventional computing altogether [1, 2]. We develop a new Data-Driven framework capable of predicting wave propagation in viscoelastic solids directly from in-situ Dynamic Mechanical Analysis (DMA) data, without the need for regression or modeling of the data. Specifically, we formulate the problem in the frequency domain and seek to minimize a distance between physically admissible histories of stress and strain, in the sense of compatibility and equilibrium, and DMA data. Following [3], we find that the natural distance that metrizes the space of histories in the frequency domain is the Wasserstein distance from optimal transport theory [4]. The great advantage of the Wasserstein distance is that it naturally interpolates between frequencies and allows the response of the system at one frequency to be inferred from data at nearby frequencies. We demonstrate and verify the approach by means of selected test cases, with particular focus on convergence with respect to the data. As an illustrative application, we apply the approach to the simulation of neuromodulation of the human brain directly from patient-specific in situ Magnetic Resonance Elastography (MRE) data.

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Distance Minimizing based Data-Driven Computational Method for Elasto-plastic Analysis with Fixed Dataset

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Key Words: *distance-minimizing, fixed dataset, multi-level K-d tree, data supplement method, fixed dataset, elasto-plastic analysis*

Abstract

The model-free distance-minimizing data-driven computational method has recently become a novel paradigm for solving various mechanics problems. With this paradigm, boundary-value problems can be solved with a discrete constitutive dataset. However, the paradigm may suffer from low efficiency since tremendous iterative searches of key data points in the discrete dataset are needed during the solution process and the mechanical behaviors of history dependent materials cannot be represented purely by a fixed dataset. To accurately and efficiently solve the elasto-plastic deformation problems with the paradigm in our work, on the one hand, the multi-level K-d tree and data supplement method are developed for effective data addition and fast data search, on the other hand, the fixed dataset considering path dependent behaviors of materials is constructed. With this kind of fixed dataset, a stress correspondence method is developed to compute the plastic strain of every integration point at each load step, and a data-driven classification model for yielding is constructed to rapidly determine the yield status of each integration point in the method. Moreover, a symmetric mapping method is developed to accurately determine the stress-strain state for the integration points under unloading or inverse loading with the fixed dataset. Results of some representative numerical examples of plastic deformation problems demonstrate that the method possesses high accuracy and efficiency. This work was supported by the NSFC (Nos. 12072062 and 12072061), the LiaoNing Revitalization Talents Program (XLYC1807193), Key Research and Development Project of Liaoning Province (2020JH2/10500003) and Fundamental Research Funds for the Central Universities (DUT20LAB203).

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EUCLID (Efficient Unsupervised Constitutive Law Identification and Discovery): Application to Plastic Hardening

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Key Words: *Unsupervised, Sparse Regression, Constitutive Models, Elasto-Plasticity*

We recently proposed a new approach for data-driven automated discovery of constitutive laws in continuum mechanics called EUCLID (Efficient Unsupervised Constitutive Law Identification and Discovery) [1]. The approach is unsupervised, i.e., it requires no stress data but only displacement and global force data, which are realistically available through mechanical testing and digital image correlation techniques; it delivers interpretable models, i.e., models that are embodied by parsimonious mathematical expressions discovered through sparse regression of a large catalogue of candidate functions; it is one-shot, i.e., discovery only needs one experiment - but can use more if available. The method was successfully demonstrated for discovering hyperelastic strain energy density functions [1,2] as well as perfectly plastic yield functions. As plastic yield functions in general depend on the loading history, i.e., the material behaviour cannot be assumed as perfectly plastic, the goal of the current work is to consider the effects of hardening in the discovery procedure. To this end a large catalogue of candidate yield functions and hardening laws is formulated. Then a sparsity promoting optimization problem, which enforces local equilibrium constraints in the bulk and global equilibrium constraints at the loaded boundary of a deformed specimen, is solved to select the yield surface and hardening law that both fit the given data and are described by concise interpretable mathematical expressions.

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Experimental Validation of the EUCLID approach for Unsupervised Discovery of Hyperelastic Constitutive Laws

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Key Words: Constitutive models; Experimental validation; Hyperelasticity; Interpretable models; Inverse problems; Sparse regression; Unsupervised learning;

We validate experimentally the data-driven approach for the automated discovery of isotropic hyperelastic material laws proposed in [1] and termed *EUCLID* (Efficient Unsupervised Constitutive Law Identification and Discovery). The approach only requires displacement and global force data and delivers interpretable models, i.e., models that are embodied by parsimonious mathematical expressions discovered through sparse regression from a large catalogue of candidate functions. The problem of unsupervised discovery is solved by enforcing equilibrium constraints in the bulk and at the loaded boundary of the domain. Sparsity of the solution is achieved by ℓ_p regularization combined with thresholding, which calls for a non-linear optimization scheme whose hyperparameters are partially determined by imposing physics-based constraints.

In the original paper, the approach was demonstrated on artificial results obtained by finite element computations. Here, we aim at its validation using experimental data. To this end, mechanical tests are performed on different rubber specimens with increasing geometrical complexity, so as to locally promote a multiaxial stress state. The displacement field is measured with digital image correlation (DIC), while the applied global force is monitored using a load cell. The effect of the geometrical complexity and of the DIC spatial and temporal resolution is investigated. Then, the obtained laws are used to predict an additional experimental test not involved in the discovery phase.

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Inverse identification of cyclic constitute law of structural steels using Bayesian optimization

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Key Words: *Elastoplastic Constitutive Law, Cyclic Loading, Bayesian optimization*

Accurately modeling cyclic elastoplastic behavior of structural steels is essential to establish reliable structural analysis results, especially for structural systems under earthquake excitations that commonly behave in a ductile manner. However, the identification of the underlying material parameters to simulate such behavior is very difficult because cyclic material tests are not usually available. Therefore, structural responses may be used for identification. Moreover, performing many nonlinear response history analyses or static cyclic elastoplastic analyses demands substantial computational cost. The dataset-specific bias has also not been fully addressed by the current identification methods.

To address this issue, this work proposes using Bayesian optimization (BO) [1] for solving an inverse problem by which certain parameters of the nonlinear combined isotropic/kinematic hardening model for structural steels are inferred from responses of a specimen or structure tested under cyclic loading. In this way, BO minimizes an error function that represents the difference between simulated responses and those measured experimentally, while providing a global-optimization framework for the identification and considerably reducing the number of simulation calls.

BO first creates a training dataset of different samples of material parameters and the corresponding error function values using a detailed finite element model of the experiment and the experimental measures. A Gaussian process model is constructed based upon this training dataset to produce a predictive model of the error function for a set of parameters. This model is then used for developing an acquisition function that intelligently guides BO during the search process by balancing exploration and exploitation of the parameter space.

Identification results from cyclic tests of a steel specimen show that the parameters identified by BO well reproduce the hysteresis behavior of the steel subjected to different cyclic loading conditions. Experimental results from different loading histories are also recommended to be utilized for the identification to mitigate the bias toward a specific load pattern that may lead the identified parameters to inaccurate predictions of the material behavior subjected to other load cases.

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Machine learning constitutive models of inelastic materials with microstructure

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Abstract

Traditional simulations of complex mechanical deformation are technologically crucial and computationally expensive. Developing comparably accurate models directly from data with lower computational cost can enable more robust design, uncertainty quantification, and exhaustive structure-property exploration. We have been developing neural network models that are guided by traditional constitutive theory, such as tensor function representation theorems to embed symmetries, and also exploit deep learning to infer intrinsic microstructural features. Neural networks are flexible since sub-components of their graph-like structure can be arranged to suit particular tasks, such as image processing and time integration. This talk will describe the architecture and demonstrate the efficacy of neural networks designed to model the response of elastoplastic and viscoelastic materials with pores, inclusions or grains based solely on observable data.

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Mechformer: A General Deep Learning Model for History-Dependent Mechanical Response Prediction

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Abstract: The traditional computational prediction of nonlinear history-dependent mechanical responses subjected to random excitation sequences suffers laborious manual modelling and unsatisfactory accuracy with low computational efficiency. In this paper, we propose a general deep learning model named *Mechformer* (**Mech**anical Trans**former**), which is able to efficiently reproduce the history-dependent mechanical responses with high fidelity under any loading protocols. First, we analyze and abstract the distinctive traits of the history-dependent mechanical response simulation: ultra-long sequence, significant memory effect, and causal autoregression. Upon these inductions, we introduce the Transformer architecture predicated on an advanced fast attention mechanism and further incorporate reversible network technique as well as GRU (gated recurrent unit), which manage to extract global historical information at any distance with linear algorithmic complexity. Moreover, to address arbitrary mechanical inputs, a new data normalization method named *NRVS* (**N**onlinear **R**eference-**V**alue **S**caling) is presented. Then we perform a numerical experiment based on a sophisticated constitutive model of low-yield-point steel featuring strong nonlinearity and strain range dependence effect. The results demonstrate the effectiveness, high efficiency, and excellent generalization capability of our developed model in reproducing the complicated mechanical responses, thus promising a new expressive alternative for the elaborated constitutive modelling. Finally, we discuss the mechanical interpretation of our model to facilitate a more intuitive comprehension.

Key Words: *history-dependent effect; deep learning; Mechanical response; Transformer; attention mechanism; intelligent design*

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Neural Network-Based Constitutive Model for Solid Materials

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Key Words: Neural Network, Constitutive Modelling, Plastic Deformation, Damage Mechanics

Constitutive models have been utilized to study the mechanical behaviors of solid material. The formulation of constitutive relations is difficult and could be associated with limiting hypothesis. In recent years, machine learning techniques have shown promising capabilities for capturing material behavior [1][2]. This work proposes novel neural network-based approaches to reproduce the complex nonlinear constitutive relations of solid materials including elastic behavior, plastic deformation and damage mechanism. A history-based strategy has been suggested using an artificial neural network for training path-dependent inelastic behavior. The network development is based on a general internal variable formalism. The number of selected internal variables is linked to the problem and degree of accuracy.

It is shown that the proposed methodology can represent exactly the von Mises elastoplastic material model in uni-axial stress state. The strategy was applied to sequences of training and validation data which were generated numerically for elastoplasticity with and without hardening as well as for elastoplastic damage. The results have been compared against established mathematical models and shown a potential of describing complex non-linear solid material behavior accurately in one-dimensional and multi-dimensional space.

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Physics-informed neural-operator for multi-scale mechanics and materials

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Abstract

The macroscopic behavior of materials that we observe and exploit in engineering applications results from complex interactions between physics at multiple lengths and time scales: electronic, atomistic, domains, defects, etc. Multiscale modeling seeks to understand these interactions by exploiting the inherent hierarchy where the behavior at a coarser scale regulates and averages the behavior at a finer scale. Such an approach can be challenging for two reasons. First, it is computationally expensive due to the need to repeatedly solve the finer scale model. Second, it requires a priori (empirical) knowledge of the aspects of the finer-scale behavior that affect the coarser scale (order parameters, state variables, descriptors, etc.). We address these challenges in a two-scale setting where we regard the solution of the fine-scale model as an operator (mapping between Banach spaces) and introduce a general framework for the data-driven approximation of such operators with the capacity of incorporating universal physics principles. This approach results in a physics-informed neural operator approximation that is computationally inexpensive, resolution (mesh) independent, and can be used directly in the coarser scale computations. Furthermore, we show that the physics-informed neural operator is capable of dramatically decreasing the amount of data required for learning the true material behavior compared to a pure data-driven setting.

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Polyconvex Anisotropic Hyperelasticity with Neural Networks

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Key Words: constitutive modeling, nonlinear elasticity, anisotropic hyperelasticity, physics-informed machine learning, input convex neural networks

In the present work [1], two machine learning based constitutive models for finite deformations are proposed. Using input convex neural networks, the models are hyperelastic, anisotropic and fulfill the polyconvexity condition, which implies ellipticity and thus ensures material stability. The first constitutive model is based on a set of polyconvex, anisotropic and objective invariants. The second approach is formulated in terms of the deformation gradient, its cofactor and determinant, uses group symmetrization to fulfill the material symmetry condition, and data augmentation to fulfill objectivity approximately. The extension of the dataset for the data augmentation approach is based on mechanical considerations and does not require additional experimental or simulation data.

The models are calibrated with highly challenging simulation data of cubic lattice metamaterials, including finite deformations and lattice instabilities. A moderate amount of calibration data is used, based on deformations which are commonly applied in experimental investigations. While the invariant-based model shows drawbacks for several deformation modes, the model based on the deformation gradient alone is able to reproduce and predict the effective material behavior very well and exhibits excellent generalization capabilities. In addition, the models are calibrated with transversely isotropic data, generated with an analytical polyconvex potential. For this case, both models show excellent results, demonstrating the straightforward applicability of the polyconvex neural network constitutive models to other symmetry groups.

Finally, we also extend the physics-guided neural network constitutive models towards inelastic and multiphysical material behavior.

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Polyconvex material models using Neural ODEs

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Key Words: Machine learning, Nonlinear elasticity, Constitutive modeling, Skin mechanics

Data driven methods are becoming increasingly prevalent in many scientific applications including constitutive modeling of materials. It has been shown that neural network based material models can learn complex material response without the limitations of expert-constructed analytical models. All material models must satisfy a set of physics-based constraints such as polyconvexity of strain energy [1]. However, satisfying this condition in a data-driven approach is difficult. The most common approach to tackle this problem so far has been to simplify the problem by replacing the polyconvexity of strain energy with a more tractable condition such as convexity of strain energy with respect to the Green deformation tensor. Then neural networks are trained with loss functions that penalize nonconvex outputs.

While this approach may succeed under certain conditions, it is an approximate method and has a limited scope. There is no guarantee that the strain energy will be convex anywhere, especially outside the training region. The loss functions that are used to train neural networks in this approach also result in highly nonlinear loss spaces which in turn makes the training very difficult.

In this study we develop a data-driven material model that satisfies polyconvexity of strain energy a priori [2]. For this we employ a new type of neural networks known as neural ODEs [3] to estimate derivatives of the strain energy function with respect to invariants of deformation. In the current approach the strain energy derivatives are defined as the solution of a neural ODE at some fictitious time $t = 1$. Since the solutions of an ODE at any given time are monotonic this results in an automatically convex function.

We train the neural ODE using experimental data from porcine skin and synthetic data generated from popular closed-form models. We show that the neural ODE is able to learn and replicate the outputs of all the closed-form models and outperforms the models when trained with experimental data. We implement the neural ODE based material model in a finite element method software to test and showcase its use in practical applications.

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Real Time Hyper-elastic Simulations with Probabilistic Deep Learning

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Key Words: Bayesian Inference, Deep Learning, Hyperelasticity, Finite Element Method, Real Time Simulation

Computer simulation has acquired a preeminent role in recent years, particularly, many engineering applications rely on the predictive capabilities of computational models. Some of these applications, like biomedical simulations used to support or train surgeons [1][2] require computationally efficient or even real-time solutions. Conventional methods for solving the underlying non-linear problems, such as the Finite Element Method, are computationally far too expensive. This work efficiently leverages state-of-the-art data-driven techniques to give accurate non-linear solutions in real-time.

In this work, we propose a highly efficient deep-learning surrogate framework that can predict deformation responses of hyper-elastic bodies under external loads. We implement a special type of convolutional neural network (CNN) [3], the so-called U-Net. This architecture has strong resemblances to Finite Element multigrid methods and proves to be capable of capturing non-linear responses characteristic to large deformation regimes. We train variants of U-Net with synthetic force-displacement data generated with the finite element method. In addition to the standard deterministic version of the framework, we propose its probabilistic versions, which can provide reliable uncertainty estimates of U-Net models in addition to predictions. We study the properties of frameworks for several benchmark problems. In particular, we check the capabilities of the Maximum Likelihood and the Variational Bayes Inference [4] formulations to assess the confidence intervals of solutions.

The use of the U-Net surrogate model allowed us to gain x350 speedup, enabling us to achieve real-time responses. The solution errors of the surrogate model have been shown to correlate with the uncertainties predicted by the proposed probabilistic framework. We also show that uncertainties of solution rapidly increase in the extrapolated region [3]. With our framework we could assess both: model and data uncertainties, which we believe is an important step towards making real-time hyper-elastic simulations more reliable.

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Surrogate model of elastic large-deformation behaviors of compliant mechanism using co-rotational beam element

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Key Words: Compliant mechanism, Large-deformation analysis, Surrogate model, Co-rotational beam element

In this study, we propose a surrogate model for predicting nonlinear structural deformations of elastic flexural mechanisms. Psuedo-rigid-body model is often used for describing the behaviors of a structure, such as compliant mechanism, with deformation degrees-of-freedom (DOF) as a combination of rigid bars and torsion springs [1]. However, it is necessary to construct a computational model based on the geometrical shape of each structure by trial and error.

In accordance with Ref. [2], by using co-rotational beam element, we develop a generalized surrogate model, which can predict nonlinear responses of a compliant mechanism with the essential deformation DOF of beam element without any geometrical assumption. The total number of DOFs of nodes at both ends of a two-dimensional beam is six, while the number of deformation DOFs is three, i.e., axial extension, symmetric bending, and anti-symmetric bending. Therefore, it enables us to reduce the computational cost, from 6×6 to 3×3, associated with the models by using the essential deformation DOFs of the co-rotational beam element.

It is difficult to predict the nonlinear responses of forces derived from displacements of a compliant mechanism represented by a co-rotational beam element. The reason is that a single forced-displacement simulation can produce multi-stable states due to the geometrical nonlinearities and numerical instabilities. To overcome this problem, we generate the data sets by applying external forces and use its inverse response for training the surrogate model.

In the numerical examples, large-deformation behaviors of several types of compliant mechanisms are predicted by the proposed model. The accuracies of the prediction are investigated for verifying that it can be a beneficial tool for designing structures with nonlinear elastic deformation behaviors.

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Surrogate models for full-field prediction of stress and fracture of fibre reinforced composites

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Key Words: *Convolutional Neural Networks (CNNs), Phase-field fracture, FFT method*

Fibre reinforced composites are important structural materials in various industrial sectors. The optimised design and certification of such materials rely on efficient multiscale analysis. Physics-based models, described by partial differential equations (PDE), have been subject to intensive research since several decades, and have enabled high-fidelity simulations providing accurate predictions of the mechanical behaviour of composites. However, these PDE solving simulations suffer from limitations in computation time, especially when it comes to composite design and certification where a large number of simulations are required to cover the parameter space. Machine learning techniques have step-changing potential, accelerating the prediction by several orders of magnitudes [1]. This is particularly interesting in the context of multiscale computations.

In the present work, an FFT (Fast Fourier Transform) based phase-field model [2] will be applied to predict the elastic behaviour and failure of fibre-reinforced composite RVEs (Representative Volume Elements). Harnessing the efficiency of the FFT method in parallel computing, a large dataset of high resolution (250,000 elements) can be obtained in a reasonably short time. FFT methods rely on image-type (uniform structured) discretisation, which makes it relatively straightforward to apply Convolutional Neural Networks (CNNs) to the obtained dataset.

The aim is to predict not only the full stress-strain curves up to final failure, but also the local stress distribution and crack patterns. The latter are important for multiphysics problems to predict the interactions between mechanical fields (including damage) and environmental factors, such as hydraulic pressure and oxidation. Both geometric variations (e.g. fibre arrangement, void distribution) and material variations (e.g. inhomogeneous matrix properties) will be included in the parameter space. Several CNN architectures will be examined and compared. Auto-encoders will be tested as a technique for dimension reduction. Networks, such as Generative Adversarial Networks, will be tested for predicting the local stress and damage fields.

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Unsupervised discovery of interpretable linear viscoelastic constitutive laws

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Key Words: Unsupervised learning, Linear viscoelasticity, Sparse regression

We extend the new approach for data-driven automated discovery of material laws, called EUCLID (Efficient Unsupervised Constitutive Law Identification and Discovery) [1], to linear viscoelastic materials. The approach is unsupervised, i.e., it requires no stress data but only full-field displacement and global force data. However, should stress-related data be available, as in the case of DMA data, the method is able to incorporate them in the discovery process. For linear viscoelastic materials, EUCLID discovers parsimonious material parameters through sparse regression of a potentially large catalogue of parameters. The material model library is constructed by using a Prony series in the frequency domain. The selection of the parsimonious parameters within the catalogue is made by solving an optimization problem that enforces the equilibrium constraints and, if available, exploits the DMA data. Sparsity promoting regularization is used to generate a set of solutions out of which the solution with lowest cost and highest parsimony is automatically selected. Through virtual experiments, we demonstrate the ability of EUCLID to accurately discover several linear viscoelastic materials.

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Coupling Separable Monte Carlo with Kriging-based Adaptive Reliability Analyses in High Dimensional Problems

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Key Words: Structural Reliability, Machine Learning, Separable Monte Carlo, High dimensional problems

In the context of reliability, adaptive surrogate model-based approaches are receiving growing interest. The classical sampling-based method - Monte Carlo (MC) - used to compute failure probabilities requires a large number of evaluations of often complex and numerically expensive models. In order to reduce the overall computational burden two paths are generally followed: (1) by introducing a surrogate model or (2) adopting a sampling strategy able to reduce the number of samples of the complete model to achieve a targeted precision. In this work, we couple both alternatives with the aim of solving reliability problems with high dimensional uncertain variables. Indeed, real world engineering problems generally involve a large number of variables, making the surrogate modeling more challenging. In this work, we adopt an adaptive Kriging- Partial Least Square (KPLS) model [1], specifically introduced to deal with high number of input variables. This is coupled with a variance-based stopping criterion [2] and Separable Monte Carlo (SMC) approach [3], designed for applications where the systems exhibit independent response and capacity.

A high dimensional numerical test case, related to structural reliability, is presented. To achieve the same accuracy level, the presented approach can reduce by 50% (if coupled with MC) to 75% (if coupled with SMC) the number of full model evaluations, compared to analogue existing methods in literature.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Multi-fidelity modeling of multi-scale porosity defects in cast alloys

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Key Words: *Multiscale simulation, Gaussian processes, multi-fidelity modelling, cast alloys.*

Cast alloys often contain heterogeneous pores that significantly affect alloy behavior in high-performance applications. To understand the cross-scale impact of microscale porosity characteristics on the cast component's macro-mechanical properties, expensive multi-scale simulations are typically required. In this talk, we will introduce a multi-fidelity and multiscale framework to simulate the behavior of metallic components containing process-induced pores. Major components of our approach include: (1) a porosity-oriented 3D microstructure reconstruction algorithm which mimics the material's local heterogeneity, (2) a novel mechanistic reduced-order model which significantly reduces computational costs by projecting solution variables into a lower dimensional space where the material's elasto-plastic behaviors are approximated, and (3) a novel multi-fidelity method based on latent-map Gaussian processes that streamline assimilating any number of data sources with variable fidelity level.

Sensitivity-free Topology Optimization using Stochastic Gradient Estimators

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Key Words: *Topology Optimization, Reinforcement –learning, Sensitivity analysis, topology optimization for crash-worthiness*

Sensitivity analysis is an essential element of current topology optimization methods. It usually takes the form of the derivative of the objective function with respect to the design parameters, and as such, it allows to guide the optimizer updating the design. However, for the objective functions which cannot be differentiated, obtaining the sensitivities becomes difficult. So far, the common approach was to approximate the objective with another differentiable function, such that the sensitivities can be still obtained by differentiation. However, designing such an approximation is oftentimes problem-specific, and comes with shortcomings due to the intrinsic nature of approximations.

Here, we propose an alternative approach inspired by reinforcement learning, where the optimizer does not have access to the derivatives of the objective, but instead it estimates the sensitivities by interacting with the model. This results in a non-intrusive topology optimization method, which no longer requires the user to provide sensitivities, but instead, estimates the sensitivities implicitly by interacting with the model of the objective. In other words, the sensitivity analysis becomes completely separated from the problem and is fully taken care of by the optimizer. The optimizer can be therefore plugged in ‘as-is’ to any physical model and does not require manually engineered approximations and sensitivity schemes.

We present our approach on several examples with differentiable and non-differentiable objectives and compare our method with the community standards.

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Application of evolutional deep neural network to external flows

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Key Words: Neural Networks, Wake, Simulation

Computational fluid dynamics plays an important role in understanding complex flow phenomena. However, it is widely known that grid generation and adaptation are bottlenecks that hamper computational efficiency and scalability. For example, configurations that feature dynamic vortex shedding and evolution require careful grid generation to resolve separation events and dynamic grid refinement to capture the evolution of shed vortices. Therefore, we always encounter the trade-off relationship between the computational cost and accuracy of the simulation. To ease the burdens of conventional numerical approaches, supervised machine learning-based surrogate modeling has been actively proposed in recent years. For instance, a machine-learned turbulent inflow generator can produce the turbulent channel flow with much lower computational cost than the corresponding driver simulation [1]. In addition, supervised machine learning is utilized to enhance the resolution of coarse resolution simulation [2]. Despite the growing adoption of supervised machine learning among the fluid dynamics community, preparation of sufficient and refined training data using numerical simulation is an eternal challenge for supervised machine learning.

To overcome the aforementioned data preparation issue, an *Evolutional Deep Neural Network* (EDNN) has been devised [3]. Given only the initial/boundary conditions and governing equations, EDNN can produce temporal evolution of the flow by evolving the parameters of the network. Therefore, there is no need to prepare training data at all. In the original study, prediction of various canonical flows is demonstrated and EDNN shows notable producibility of flows in long-time prediction.

In this study, as a next interest, we focus on representing an external flow embedding a bluff body by EDNN. More concretely, the flow around a circular cylinder is considered. The predicted flow field at Re=40 shows agreement with reference direct numerical simulation (DNS). In the talk, we will show statistical assessments and dependence on the Reynolds number.

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Development of AI Diagnosis of Cracks in Concrete Structures Using Digital Hammering Inspection

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Key Words: *Non-destructive Testing, Concrete, Crack, Artificial Intelligence, Hammering test*

Visual inspection and hammering inspection are widely used as conventional inspection methods for cracks in concrete structures due to its capability to investigate a huge number of inspection targets in a short time. On the other hand, these methods depend on the experience and skills of the inspectors, and it has been pointed out that these skills are not easily transmitted.

Under such a background, a hammering inspection using a sensor (hereinafter referred to as "digital hammering inspection"[1]) has been developed for the evaluation of cracks in concrete structures objectively. However, it is difficult to comprehensively understand the influence of cracks on the digital hammering inspection, because the shapes of cracks (depth, length, direction, etc.) are diverse in actual structures.

Therefore, in this study, we developed a technique to quantitatively evaluate the shape of cracks from the results of 2-dimensional planar ditigal hammering inspection in the following two steps.

(1) Construct a large-scale DB of various concrete crack shapes and the 2-dimensional digital hammering inspection results using FEM analysis and machine learning.
(2) Develop an inverse analysis model to estimate the crack shapes from the planar inspection results by machine learning the obtained DB.

The developed inverse analysis model showed that the crack shape can be estimated with an accuracy of about ±15% by learning the nonlinear relationship between the digital hammering inspection results and the database of crack shapes. However, since the developed inverse analysis model is limited to the evaluation of a single crack in the concrete structures, we are planning to extend its applicability to actual cases in the field by learning the data of multiple cracks.

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Local Extreme Learning Machines for Computational PDEs: Algorithm and Comparison with Classical and High-Order Finite Elements

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Key Words: *Randomized neural networks, Scientific machine learning, Extreme learning machine, Nonlinear least squares method*

Existing deep neural network (DNN) based methods for solving boundary/initial-value problems suffer from several drawbacks (e.g. limited accuracy, general lack of convergence with a certain convergence rate, extremely high computational/training cost) that make them numerically less than satisfactory and computationally uncompetitive.

We present a neural network-based method for computational PDEs that largely overcomes the above drawbacks. This method, termed local extreme learning machines (locELM), combines three ideas: extreme learning machines, domain decomposition, and local neural networks. The field solution on each sub-domain is represented by a local feed-forward neural network, and C^k continuity conditions are imposed on the sub-domain boundaries. The hidden-layer coefficients of the local neural networks are pre-set to random values and fixed, and only the output-layer coefficients are trainable parameters. The overall neural network is trained by a linear or nonlinear least squares computation, not by the back propagation (or gradient descent) type algorithms.

The presented method exhibits a clear sense of convergence with respect to the degrees of freedom in the neural network. Its numerical errors decrease exponentially as the number of degrees of freedom (e.g. the number of trainable parameters, number of training data points) increases, which is reminiscent of the traditional high-order methods. The current method far outperforms the state-of-the-art DNN based PDE solvers (e.g. the deep Galerkin method, and the physics informed neural network method) in terms of the accuracy and computational cost (network training time). We compare systematically the computational performance of the current method with those of the classical 2^{nd}-order and high-order finite element methods (FEM) for solving linear and nonlinear PDEs. The current method far outperforms the classical FEM. Its computational performance is comparable to that of the high-order FEM for smaller problem sizes, and for larger problem sizes the current method markedly outperforms the high-order FEM.

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Neural network based isogeometric design space exploration

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Key Words: *Neural Networks, Design Space Exploration, Isogeometric Analysis*

The projected increase in computational resources in the coming decades will pave the path for a fast, direct, interactive, and real-time approach for design space exploration of industrial problems. The traditional design space exploration approaches suffer from a design-through-analysis bottleneck that involves a significant user time commitment and prohibits real-time design space exploration. The isogeometric design space exploration framework proposed in [1] overcomes this is issue by leveraging concepts from isogeometric analysis (IGA), which provides seamless integration between FEA and CAD, with modern parametric modeling techniques and efficient design space sampling. The heart of this approach involves traditional approximation methods, such as modal and nodal approaches, for constructing an efficient mapping between design parameters and the solution manifold consisting of IGA control points. However, these parametric modeling methods suffer from the curse of dimensionality that limits them to a lower order of accuracy in a high dimensional parametric space.

In this presentation, we propose to use neural networks as a surrogate model to represent the mapping between high dimensional input design space and the solution manifold. Neural networks allow for an efficient and accurate representation of a high dimensional parametric space that does not suffer from the curse of dimensionality as other previously considered parametric approaches. We plan to test the limits of nodal, modal, and neural-network-based surrogate models by evaluating them for scenarios inside and outside the training design space for several structural mechanics problems. The overarching goal is to assess the performance of these methods for representing solution manifolds with rough characteristics as these problems are often challenging for traditional approaches.

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Physics Guided Deep Learning Method to Surrogate Flow Simulation

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Key Words: Deep Learning, Surrogate Model, Computational Fluid Dynamics

The application of deep learning to physics simulation has been addressed, and it is expected to reduce calculation costs by surrogating simulations, resulting in faster optimization calculations and more efficient design processes. Usual deep learning algorithms, however, don't take into account governing equations of physical simulations in the training process. Therefore, the predicted physics fields don't always satisfy the governing equations, which is one of the reasons why many researchers think these methods is not suitable for practical use. In our research, we focused on physics-guided learning[1], which considers the residuals of the governing equations in the loss function. This method is verified its effectiveness by applying to cavity flow, which is 2D incompressible flow simulations.

Different data were used for the training and the inference test. Target physicsal quantities are pressure, x and y components of velocity. The evaluation metrics such as mean absolute percetage error and residual were compared between usual deep learning and physics-guided learning. Residual of Navier-Stokes equation, which is governing equation of cavity flow, are computed by substituting the derivatives of inferred pressure and velocity field. The result revealed that although usual deep learning model seem to predict pressure and velocity fields well, the residual are relatively large. This is due to the roughness of inferred pressure field. On the other hand, physics-guided learning can predict pressure field smoothly, resulting in the residual is improved significantly. From the above, it is found that the inferred physical fields are smoothed by physics-guided learning and the effectiveness of physics-guided learning is confirmed.

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Physics Informed Neural Networks for Heterogeneous Materials

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Key Words: *PINNs, Deep learning, Heterogeneous materials, Hyperparameter sensitivity*

High-fidelity physics-based numerical models have often been utilized for subsurface modeling in the oil and gas industry. These models provide an efficient virtual platform to investigate the various operational parameters and guide on-field engineering decisions. The thermo-hydro-chemo-mechanical interactions in the subsurface processes are incorporated by means of coupled-field balance laws in these models. The resulting equations are discretized and then solved on a computer using a fit-for-purpose numerical method. However, all numerical methods require that the subsurface system be appropriately meshed into non-overlapping elements. Unfortunately, generating such meshes for subsurface systems is a non-trivial task. This is because most subsurface systems are geometrically complex and exhibit a high degree of heterogeneity. In addition to naturally occurring faults, and natural variation in material properties because of geological stratification, these systems also include the effect of fractures engineered through hydraulic stimulation. Consequently, the pre-processing step of generating conforming meshes that honor the various subsurface features adds an enormous computational burden. An appropriate discretization scheme is then chosen to compute the derivatives and other terms in the equations. This introduces discretization errors and could potentially lead to stability issues.

On the other hand, data-driven modeling approaches use large artificial neural networks to predict the outcome of physical systems. The training data for these models is generated by means of physics-based simulators (or experiments) for simpler models. Once trained, the artificial neural network is expected to mitigate the high computational cost of physics-based simulators through fast predictions. However, in practice, the outcome of these data-driven simulations is only as good as the training data. Often, the cost of training data acquisition is prohibitive and severely limits the applicability of these methods.

To address the above limitations, a novel class of methods known as the Physics Informed Neural Networks (PINNs) is increasingly becoming popular. These methods take a hybrid approach between purely physics-based and purely data-driven modeling by constructing loss functionals based on underlying physical principles. In contrast to the more traditional numerical methods, PINNs are not mesh-based and therefore obviate the need for mesh generation and discretization, while allowing the derivatives to be computed exactly using automatic differentiation. At the same time, in contrast to traditional data-driven methods, PINNs are guided by underlying physical principles and are therefore more computationally efficient. With a few exceptions, PINNs have so far been applied only for homogeneous materials. Here, we explore the applicability of the PINNs framework to materials with a heterogeneous character. Through simple 1D and 2D benchmark examples, an exhaustive parametric sensitivity study is conducted to isolate the effect of hyperparameters and activation functions on the numerical performance of the method. Through these examples, it will be demonstrated that the choice of activation functions has a significant impact on the convergence of the method for problems with material interfaces.

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Bayesian Optimization on Fifth-Order Targeted ENO Scheme for Compressible Flows

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Key Words: Bayesian Optimization, Targeted ENO, Implicit Large Eddy Simulation

Targeted ENO (TENO) has originally been proposed by Fu et al. [1] in order to overcome the shortcomings of WENO schemes which are excessive dissipation, and limited robustness for lower order upwind-biased, and central-biased schemes, respectively [2]. TENO offers a set of free parameters to alter the inherent effective local dissipation and dispersion. In the original formulation of [1], these free parameters have been adjusting by means of the approximate dissipation-dispersion relation [3].

Data-driven methods enable optimizing these free parameters instead of adjusting these. In this work, we demonstrate the application of an iterative Bayesian optimization approach on designing fifth-order TENO (TENO5) schemes. Exploiting that Bayesian optimization efficiently and robustly finds an optimum of an expensive function with a low number of trials, we construct specific TENO5-schemes for compressible flows with gasdynamic discontinuities, and implicit large eddy simulation (ILES) of turbulent flows. For the former, we measure the error between under-resolved simulations of the Sod shock tube and its analytical solution for automatically generated TENO5 formulations. For the latter, under-resolved inviscid Taylor-Green vortex flows are evolved to their turbulent state, in which their kinetic energy spectrum in the inertial subrange is compared to the theoretical Kolmogorov-scaling solution.

We show that these two TENO5 formulations perform superior to the original formulation of [1] for the wave-number ranges in dissipation-dispersion relation relevant to the specific types of flows. Also, a variety of benchmark test flows show that both TENO5 formulations perform better than the original one in terms of phase speed, shock resolution and physical consistency of turbulent flows, i.e. in practical applications.

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Gaussian processes meet NeuralODEs: A Bayesian framework for learning the dynamics of partially observed systems from scarce and noisy data

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Key Words: *Scientific Machine Learning, Dynamical Systems, Uncertainty Quantification, Model Discovery*

We present a machine learning framework (GP-NODE) for Bayesian systems identification from partial, noisy and irregular observations of nonlinear dynamical systems. The proposed method takes advantage of recent developments in differentiable programming to propagate gradient information through ordinary differential equation solvers and perform Bayesian inference with respect to unknown model parameters using Hamiltonian Monte Carlo sampling and Gaussian Process priors over the observed system states. This allows us to exploit temporal correlations in the observed data, and efficiently infer posterior distributions over plausible models with quantified uncertainty. Moreover, the use of sparsity-promoting priors such as the Finnish Horseshoe for free model parameters enables the discovery of interpretable and parsimonious representations for the underlying latent dynamics. A series of numerical studies is presented to demonstrate the effectiveness of the proposed GP-NODE method including predator-prey systems, systems biology, and a 50-dimensional human motion dynamical system. Taken together, our findings put forth a novel, flexible and robust workflow for data-driven model discovery under uncertainty.

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A Deep-Learning-Based Inverse Design Framework using Compressed Simulation Data for Self-Oscillating Gels

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Key Words: Soft Robotics, Stacked MLP, Tensor Decomposition, Inverse Design

We consider data-driven design of soft robots using a novel locomotion mechanism based on a reaction-driven motion of an oscillating sheet. While a forward model for the simulation of this sheet is available as a PDE solver by Alben et. al (2019), design applications require the inversion of sheet motion into geometric and reaction parameters of the sheet. While PDE constrained approaches for this inversion is possible, they may be time consuming and computationally expensive. Instead we develop a deep-learning based model mapping sheet motion to sheet parameters. This framework is based on a stacked MLP design, whose hyperparameters we carefully tune to reconstruct the geometric and reaction parameters with high accuracy. However, this approach to train an inverse design framework for self-oscillating gels requires a large amount of data, which both makes training demanding and slows down the training procedure. To tackle these types of challenges in more general inverse-design settings, we investigate compact representations of the simulation data through low-rank matrix and tensor decomposition methodologies on different network structures. We compare the compressed-data inverse design framework with our original framework in terms of estimation accuracy of the continuous and discrete gel-sheet parameters, training speed, and memory requirements.

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Robust Deep Learning Models for Inverse Design of Complex Mechanical Metamaterial Structures

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Key Words: GANs, Inverse problem, FEM, Metamaterials

With the advancement of additive manufacturing technologies in the recent past, rational design of human-made materials comprising of several unit cells or subunits have allowed us to program their structural response in a desired way. Extraordinary functionalities in such metamaterials can be engendered by suitably selecting the structure and geometry of the unit cells, rather than their material composition. These mechanical structures can be used for applications like soft robotics and adaptive structures, where designers can use programmable metamaterials architectures to generate complex sequence of output motions from a simple load input on a monolithic system [1]. These unique structures encompass a vast design space that cannot be possibly explored by experimental methods. Finite Element Analysis (FEA have been widely used to predict the effective properties of different metamaterials based structures. Although these works have demonstrated the enhanced design space of such Metamaterials with myriad of potential applications, we still require to address the inverse design problem, i.e predicting a metamaterial design given a specific structural response. Topology optimization (TO) [2] has been used to solve this problem. Both gradient and non-gradient based TO algorithms have been used to address this problem. However, gradient based method requires calculating cumbersome sensitivities of the objective function, which often converges to local optimal solutions. Although gradient free techniques have yielded promising results to solve the inverse design 1roblema, they primarily suffer from high computational cost. Data Driven approaches on the other hand offer a non-iterative, general-purpose solution by modelling properties as inputs and the design as output. Deep learning methods such as Generative Adversarial Networks (GANs) are promising alternatives to predict the design given a property [3].

The objective of this work is to develop a framework that can solve this inverse design paradigm. In this study we aim to find the design of the metamaterials cantilever beam subjected to a point load at the free end, for a desired centerline displacement of the beam. We arrange the metamaterial unit cells provided by Chan et al. [4], to build a cantilever beam, whose centerline displacement is calculated using a static FEA. Naturally, the deformed beam configuration depends on the choice and the arrangement of the unit cells. To predict the design of the beam (type and arrangement of the unit cells) that could result in each centerline deformation, we adopt a GANs based approach which represents the 2D structures in the form of images. As a first step, the GAN based approach has been utilized to predict a very simple metamaterials design. To cover a more extensive design space, a novel data compression strategy is employed to allow GANs to effectively train on the data. This approach results in a in a general purpose, highly expressive, and robust strategy to design more complicated metamaterial structures. We present a thorough analysis of the design results from the approach on a large dataset (>5000 samples) collated via FEM simulations. The developed framework can be extended to predict design of beams considering structural nonlinearities.

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Deep Learning Approach to extract principal stresses from Photoelasticity Images by posing it as Classification and Regression problem

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Key Words: *Deep Learning, Digital Photoelasticity, Stress Evaluation, Stress Intensity Factor*

In mechanical testing, photoelastic and digital image correlation techniques are used to obtain stress and strain fields. The stress distribution can be visualized by an isoclinic or isochromatic fringe pattern of birefringent materials subjected to mechanical loads. So image analysis of the fringe pattern is required to get information about the direction and magnitude of principal stresses. Still, it can require very complex methods such as the phase-shifting technique or inverse analysis. Machine learning models like deep convolution neural networks (CNN) are widely used for extracting information from images by posing the problem as classification, regression, segmentation, and super-resolution problem. CNN models are easy to implement and do not require any feature extraction from images. In this work, we generate isochromatic images by considering three different mechanical loadings such as (1) disk under diametrical compression, (2) half-space under concentrated surface force, (3) Half space under uniform normal loading for various force levels, and three different modes (I, II and III) of Griffith-Inglis Cracks for various stress intensity factors. Using our own developed CNN models, we extract the force levels and stress intensity factors from the images and compare them with Alexnet. The developed program achieves 90% accuracy in classification, and 0.001 mean square error in regression of images

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Image Measurement on External Reinforced Concrete Frame Retrofitting

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Key Words: *External RC frame retrofit, image measurement, crack development*

This work participated the measurement work on a series of experiments of external reinforced concrete (RC) frame retrofitting using image analysis technique. The retrofit method adds an external RC frame along the weak direction of an RC building in order to improve the seismic resistance. The connection between the external frame and the existing frame dominates the effectiveness of the retrofitting. However, it is relatively difficult to measure the relative displacements between the external and existing frames by using conventional contact devices such as the linear variable displacement transducers (LVDTs) not only because there are multiple measurement points but also they are difficult to install in limited space. Image analysis is a relatively feasible manner to measure the relative displacements between frames.

This paper briefly presents the design of the image measurement as well as the preliminary measurement results. In addition to the relative displacement aforementioned, the measurement results also include the deformations of beams and columns of both frames, the crack development over the experiments, and the observed failure mechanism based on the image analysis measurement. The feasibility of extending the measurement to future structural health monitoring is also discussed.

Optical Principle and Accuracy Evaluation of Equilateral Prism used for Stereo Image Measurement

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Key Words: *Image measurement, 3-D measurement, Prism, Single camera, Calibration*

PPSIM is a technology that uses the refraction of a prism to shift the light to produce a perspective difference effect, so as to obtain a virtual stereo image pair in the case of a single camera shooting, and use the image to perform stereoscopic reconstruction of the object space. The proposed measurement technique is specially designed to precisely measure the shape and deformation of micro-objects, especially for studying elastic and plastic behaviors in micro region, such as the measurement of stress intensity factors at the crack tip, the measurement of the deformation field around the hole by the hole-drilling method.

The purpose of this paper is to deduce the PPSIM optics, and introduce two calibration procedures for identifying system parameters. Finally, the accuracy of parameter calibration and spatial coordinate measurement of PPSIM is verified by experiments.
According to Snell's law of refraction and vector geometry, this paper deduces the equations to convert from object space coordinates to virtual stereoscopic image pair coordinates, and vice versa. Since it does not require an iterative direct calculation process to convert the coordinates of the virtual stereo image to the object space coordinates of the measurement point, it is not only used for forward intersection analysis, but also used in the calibration process of system parameters.

There are a total of 26 system parameters including lens distortion correction parameters, camera sensor density and image distance, camera external square parameters, and internal and external orientation parameters. The system parameters can be identified with the Levenberg-Marquardt algorithm, provided that at least 9 control points are arranged whose spatial coordinated are known or their displacements in three independent directions are given.

The experimental results show that reasonable system parameters can be identified whether using control points with known spatial coordinates or four images with known rigid body displacements in three independent directions. The Levenberg-Marquardt algorithm has good stability, and all experimental examples can converge smoothly. We recommend the second calibration method because it does not require a high-precision process to prepare the test body, nor does the calibration procedure require tedious operational procedures.

The experimental results of accuracy verification show that under the condition of FOV of 30mm, the root mean square of measurement error can be controlled below 0.011mm, that is to say, the relative error is about 1/3,000. This precision is close to that of the interferometer, which is enough to confirm that PPSIM has application value in experimental mechanics research and testing.

Constitutive model of expansive soils considering the influence of the cation exchange on osmotic pressure

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Key Words: *Constitutive model, Expansive soil, Cation exchange, Osmotic pressure*

The double diffusion layer of cation surrounded clay crystals yields repulsive osmotic force, and it causes mechanical deformation and/or characteristic change of soils. According to the type and concentration of solution, furthermore, those cations adsorbed on clay crystals are exchanged with other cations (the cation exchange), and it also causes mechanical deformation and characteristic change. In particular, expansive soils such as bentonite, which have large surface area and high cation exchange capacity, are strongly affected by such exchangeable cations. Bentonites are considered as artificial barrier in a waste disposal facility because of their characteristics. Buffer bentonites would be exposed to groundwater and/or seawater environments containing an inflow of sodium ions, calcium ions leached from the cement material, and iron ions from the framework of the disposal facility. This transition of the chemical environment is a significant source of concern, as it changes the expansive characteristics of the soil.

Authors proposed the constitutive model combining the behaviors of soil skeleton and clay mineral crystal based on the double structure framework[1], which can capture various complicated hydro-mechano-chemical behavior of expansive soils. In this study, introducing the fraction of adsorbed cations calculated by the Gains-Thomas convection and the Davies equation for activity coefficients of ions to the repulsive osmotic force derived from the diffusion double layer [2], the model considering the influence of cation exchange on mechanical behavior of expansive soil is established. The simulation result of the osmotic consolidation test by the proposed model, in which Na^+ ion (0.01mol/L) is initially added and subsequently Ca^{2+} ion (0.01mol/L) is added into expansive soil. The proposed model can describe the transition of osmotic consolidation phenomena with multiple ions: the osmotic force continuously changes according to the fraction of adsorbed ion; divalent ion causes larger osmotic consolidation (settlement).

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Effect of in-situ heterogeneities and pre-existing flaws on rock spalling around underground excavations

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Key Words: *spalling, heterogeneity, nuclear waste repository*

This study presents a three-dimensional numerical analysis of multiple fracture growth leading to spalling around underground nuclear waste deposition boreholes. A multiple-borehole numerical model in a heterogeneous rock mass is considered, wherein thermo-mechanical spalling is simulated using a finite element-based fracture growth simulator [1]. Fractures initiate in tension based on a damage criterion, and grow in a manner controlled by the stress intensity factors at the fracture tips. Fracture tip propagation is multi-modal, resulting in final fracture patterns that are representative of both tensile and shear failure.

Several geomechanical cases are investigated, in which spalling initiation and growth is numerically evaluated as a function of host rock heterogeneity. A first level of heterogeneity is introduced by perturbing the mechanical (strength, elastic modulus, toughness) and thermal (conductivity, heat capacity) properties, following their expected frequency distributions at the Swedish Forsmark [2,3] site. Subsequently, another level of heterogeneity is added through a large, steeply dipping fracture zone that intersects the proposed repository site [4].

The effect of spalling on the structural integrity of the deposition boreholes is illustrated for both heterogeneous cases, and quantified in terms of maximum spalling depth, spalling width, and total fractured surface area. Fracture patterns and their extent are also compared with a homogeneous benchmark case. Numerical results show that rock heterogeneity influences the propagation of spalling fractures, and their interaction with the borehole walls and the pre-existing fault, through the creation of local stress shadow zones.

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Model-Supported Assessment of Barrier Performance in Deep Geological Repositories: Contribution to the Site Selection Process in Switzerland

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Key Words: *Performance Assessment, Site Selection, Repository-induced Effects, Geological Barrier, HLW, LLW, ILW, DGR*

In the field of deep geological disposal of radioactive waste, performance assessment focuses on the integrity and performance of the engineered and geological barriers as the disposal system evolves over time. To evaluate the suitability of a site for a deep geological repository (DGR), geoscientific data is integrated into site-specific assessments for the repository project. The performance of the geological barrier needs to be evaluated based on the characteristics at the start of the assessment period (i.e., at the time of repository closure) taking into account a certain degree of uncertainty associated with the exploration and characterization of the geology as well as the long-term evolution of the site. Furthermore, performance assessment includes an evaluation of the safety-relevant repository-induced effects on the disposal system, such as thermal-, gas-, and chemical effects introduced by the interaction of the waste with the nearfield. The complexity of the involved thermo-hydro-mechanical and -chemical processes (THMC) calls for model-supported workflows to reach a quantitative assessment of the barrier performance and an adequate evaluation of the associated conceptual and parametric uncertainties.

The Swiss Radioactive Waste Management Program foresees two types of repositories: a high-level waste repository (HLW) for spent fuel, vitrified high-level waste and long-lived intermediate-level waste, and a repository for low- and intermediate-level waste (L/ILW). The procedure for selecting repository sites in Switzerland is specified in the Sectoral Plan for a DGR which consists of three stages. In the current and last Stage 3, three candidate siting regions *Jura Ost*, *Nördlich Lägern* and *Zürich Nordost* in northern Switzerland are examined in detail and, where necessary, supplementary geological investigations such as deep exploratory boreholes are being performed. The broadened site-specific database forms the basis to select, for each of the repositories, the site for which the general license application will be prepared. The model-supported workflow is developed with an indicator-based approach supporting the site selection, aimed at comparing favorable and less favorable aspects of the potential siting areas. The workflow comprises a portfolio of numerical models addressing different aspects such as the efficiency of the unperturbed geological barrier, its long-term evolution, the THMC effects from the DGR, the barrier integrity, and the spatial and temporal uncertainties in the evolution scenarios. The numerical modelling is performed with deterministic as well as probabilistic variants to bracket the conceptual, parametric, and scenario uncertainties. The assessment aspects are addressed in terms of quantitative dimensionless performance indicators for the consistent comparison of the candidate sites. The model-supported workflow allows a traceable, transparent, and verifiable implementation of the site selection process.

On The Simulation of THM Behaviour of Forge Mock-up Experiment

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Key Words: *Bentonite, Thermo-hydro-mechanical behaviour, Coupled Analysis, Unsaturated*

In the recent decades, the possible damage or deterioration of the engineered and natural barriers due to the accumulation of hydrogen and radiolysis gas with the corrosion of metals has been studied as one of the main concerns at nuclear waste disposal facilities. The FORGE project[1)] was a joint project, in which key gas migration issues on repository performance assessment was studied. In this project, a reproduction analysis of the water injection process was carried out by conducting a mock-up experiment from July 2010 to March 2013. As an engineered barrier, sand/bentonite (SB) mixture was selected, hence it is necessary to consider the swelling behavior and the permeability due to the void ratio change. Therefore, in this study, we adopted a model that can simulate the saturated swelling and elasto-plastic behavior of clay and performed hydro-mechanical coupled analysis.

The materials used in this test were mortar, bentonite and SB mixture, with initial dry densities of 1.8 and 1.5 Mg/m^3 for SB and bentonite, respectively. The thermo-hydro-mechanical (THM) coupled analysis of mock-up experiment was performed by CODE_BRIGHT[2)] with an axisymmetric model. SB and bentonite are modeled with elasto-plastic constitutive law, Barcelona Basic Model and details of the constitutive laws and parameters were explained in the report by Sakaki et al.[3)]. A mechanical condition of no displacement perpendicular to the boundary was imposed in all boundaries. Initial degree of saturation for SB was set as 0.64. Initial gas pressure of 0.1MPa was assigned to all surfaces to achieve initial equilibrium. After the initial conditions were set, two types of THM coupled analysis were performed. In the first analysis, saturation stages as applied in the experiment were set[4)] and water injection amount, water pressure and total stresses during the test were examined. In the second analysis, a simplified saturation process was applied and at the end of the analysis boundary conditions were set as simulating the dismantling process[5)]. At the end of the analysis, deformation and change in porosity were compared with the observed values due to the dismantling of the experiment.

As a result of this study, a good reproducibility of the measured water injection amount, water pressure and total stress of the mock-up experiment was obtained. Additionally, reproduction analysis could reproduce the expansion of the specimen after dismantling, and that the change in density distribution was mainly due to the expansion with dismantling. Therefore, the modelling of the water injection and dismantling processes and the validity of analysis parameters could be verified.

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A Dimension Reduction Technique to Obtain Equivalent 1D Shallow Water Equations within 2D Finite Element Framework

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Key Words: *Storm Surge, Channel Flow, CFL, Finite Element, ADCIRC*

In this presentation, we introduce a dimension reduction technique to obtain discretized equations equivalent to 1D shallow water equations within the 2D finite element method framework. The Advanced Circulation (ADCIRC) model has been used for multiple purposes including hindcasts, forecasts, and risk evaluation of hurricane storm surges [1,2]. Among other ongoing development efforts, coupling the ADCIRC storm surge model with hydrological models is one of the key focuses. Coupling of these models is especially important in the context of compound flooding, where rainwater, riverine flows, and storm surges interact to possibly cause devastative floods.
This work addresses two issues we often face when we model smaller channels/rivers within a 2D finite element framework: 1) an overly restrictive time step imposed by the CFL condition in the cross-channel direction as the cross-sectional width becomes small, and 2) poor model physics due to the use of simplified equations such as weir formula to model the exchange of water between the channel and the floodplains.

To eliminate the cross-channel CFL condition we derive discretized nodal equations in the body of the channel that are equivalent to 1D shallow water equations. The equations are obtained by manipulating the 2D finite element nodal equations at paired nodes located on either side of the channel. This technique can be implemented with significantly less effort than introducing 1D equations to the existing 2D finite element code. We address the second issue by using weir formula primarily when the water depth in the channel is below the bank elevation. We abandon these when the channel water elevation exceeds the bank elevation by a small amount and then switch instead to full integration of the shallow water equations. In this case, the channel bank represents a discontinuity in the bathymetry, and the water flow responds to the 2D physics both in the floodplain and the channel. Finally, we can combine the two solution strategies to yield a single solution that is influenced both by the floodplains as well as the along channel flow while not being restricted by a cross-channel CFL condition.

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A mesh generator for multidimensional hydrodynamic models

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Key Words: Mesh generation, Multidimensional hydrodynamic model

The computational efficiency of hydrodynamic models significantly depends on the resolution of the computational meshes employed. For regions with complex geometries, high-resolution meshes are required in order to obtain accurate results, which decreases computational efficiency. Several mesh generators have been developed to generate 2D finite element meshes with resolutions adapted for local geometric features. However, the use of two-dimensional elements alone to capture topography/bathymetry of river beds, especially when river widths are very small, can be prohibitively expense. Therefore, multidimensional (1D/2D) hydrodynamic models have been developed to address this problem in which two-dimensional elements are used for floodplains, watersheds, and lakes, while one-dimensional elements are used for small open-channels. The computational domain of the two-dimensional model is represented by triangular elements and the computational domain of the one-dimensional model is represented by edges of triangular elements. In this study, an automatic mesh generator is developed for multidimensional hydrodynamic models. One of the main features of the mesh generator is efficient mesh sizing along 1D domains, which means that resolution of elements is high around curved channels whereas it is low around straight channels. Another main feature is that it identifies small channels according to user-defined criterion and automatically extracts centerlines to be used as 1D domains. Numerical studies are performed on several watersheds and coastal floodplains with complex geometries.

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Coupling Global Ocean Circulation and Global Tide and Storm Surge Model

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Key Words: Hydrodynamics, Oceanography

The increased frequency and magnitude of tropical and extratropical storms conveys a looming need to accurately predict storm surge and flooding that result from these extreme weather events [1]. Coastal flooding can be predicted using regional models that solve the depth-averaged Navier-Stokes equations, and recent developments have allowed for such models to use global domains [4, 3]. Because these models are oftentimes purely barotropic, they fail to capture baroclinic currents such as the Gulf Stream and cannot readily resolve seasonal disparities in dissipation rates.

Recently, a study was performed that couples an regional, operational, coastal forecasting system powered by the Advanced Circulation Model (ADCIRC) for Puerto Rico and the Virgin Islands with the data-assimilated Global Ocean Forecasting System (GOFS 3.1) in order to resolve baroclinic effects within the storm surge model [2]. It was found that by using salinity and temperature information on a coarse scale from the ocean-circulation model, it is possible to capture these effects within the regional 2-dimensional model.

This study extends this coupling from a regional storm surge model to a global one. Using temperature and salinity forecasts from GOFS 3.1, estimates are found for depth-averaged baroclinic pressure gradients, Brunt-Väisälä frequencies for use in the calculation of baroclinic-barotropic energy conversion, and steric adjustments. These estimates are then used within ADCIRC to resolve baroclinic effects normally lost in depth-averaged models.

Multi-year analyses are used to examine the how the incorporation of these baroclinic effects alter the currents captured within the ADCIRC model. These results are compared with current and tidal stations to examine the differences in barotropic and baroclinic simulations.

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Development of a Fluid-Structure Interaction Method with Free Surface Using IGA

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Key Words: *Isogeometric Analysis, Fluid-Structure Interaction, NURBS*

There have been presented a number of numerical methods for fluid-structure interaction problems with free surface. The finite element method is widely used as a numerical method. Although the finite element method has excellent adaptability to arbitrary shapes, it is time-consuming to create an analysis mesh, and curves may be approximated. Therefore, IGA (Isogeometric Analysis) [1], [2] has been attracting attention in recent years.

IGA is a method using NURBS functions used in CAD (Computer Aided Design) as a shape function. IGA can create an analysis mesh directly from CAD data, enabling us to create an analysis mesh easily and represent curves perfectly.

The purpose of this study is to develop a fluid-structure interaction analysis method using IGA. For fluid analysis, the numerical method based on VOF method is employed. The stabilized finite element method with IGA is applied as the spatial discretization method and the Crank-Nicolson method as the temporal discretization method. For structure analysis, to solve the equilibrium equations, the Galerkin method with IGA is employed as the spatial discretization method and the Newmark-beta method is employed as the temporal discretization method. Several numerical examples are presented to demonstrate the promise and potential of the present method to solve the solid-fluid interaction problems with free surface.

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Gas-liquid-solid Three-phase Implicit Finite Element Analysis based on Multi-phase-field Model using Unstructured Grid

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Key Words: *Unstructured Grid, Multi-phase-field Model, Cahn-Hilliard Equation, Fluid Analysis, Implicit Finite Element Method*

An implicit mixed finite element method based on a multi-phase-field model [1] for gas-liquid-solid three-phase flow is proposed for the finite element parallel analysis. A bubble function element stabilization method [2,3] using unstructured grid (tetrahedron) is employed for incompressible Navier-Stokes equations and linear elastic body equation. Allen-Cahn equation [4] and Cahn-Hilliard equation [5,6] are applied to estimate interface of gas, liquid and solid. MINI element, bubble function element / linear element, is used to solve Cahn-Hilliard equation. As for the temporal discretization, an implicit scheme is used. In the implicit scheme, N-R method is employed to solve non-linear equations. A three-dimensional gas-liquid-solid three-phase finite element analysis is computed in this research.

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Implementation and assessment of a parametric rainfall model in a hurricane storm surge model

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Key Words: *Discontinuous Galerkin methods, hurricane storm surge, rainfall*

Current operational storm surge models incorporate several physical processes that contribute to coastal flooding; however, these models do not typically include rainfall in their storm surge simulations. This omission creates an incomplete assessment of weather conditions during extreme precipitation events and has inspired efforts to improve upon current storm surge models by incorporating rainfall into storm surge simulations. In this talk, I will explain the significance of rainfall and its contribution to storm-driven coastal flooding and discuss our efforts to integrate a parametric rainfall model into a discontinuous Galerkin shallow water equations model (DG-SWEM) to create a more complete assessment of real-life storm conditions. Numerical results demonstrating the approach will be presented, and we will discuss some of the challenges involved in moving forward.

Mechanism of delayed leaching of heavy metals from naturally contaminated soils

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Key Words: *desorption, naturally contaminated soil, porous particle, finite difference method*

Existing models for sorption kinetics of contaminants such as heavy metals (e.g., pseudo-second-order model introduced in [1]) mainly focused on describing artificial adsorption/desorption for a relatively short duration, where contaminants absorb onto the surface of the adsorbent. However, ground formed by metamorphism or sedimentation usually contains heavy metals during their natural formation process, and heavy metals are distributed throughout the ground in such cases. In fact, several research (e.g. [2]) has implied the significance of the effect of intra-particle adsorption/desorption kinetics of heavy metal leaching. From this perspective, naturally contaminated soils that contain contaminants deep within the particles may show delayed leaching. Therefore, a novel approach for predicting the distribution of contaminants, both in the soil particle and surrounding liquid, is achieved using the finite difference method. The approach is named the "intraparticle pore-diffusion model" and is applied to simulate the batch leaching test of heavy metal contaminated soils. Intraparticle diffusion and sorption equilibrium are considered. The desorption phenomena of heavy metal from soil particles are considered as a one-dimensional, polar-symmetric problem in the spherical coordinate system by supposing soil particles to be porous, perfect spheres. The results indicate that soil constituted of larger particles leach more contaminants at a certain time and faster for a certain leaching amount.

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Modeling, Simulation and Visualization of Tsunami Using Virtual Reality Technology for Disaster Mitigation Education

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Key Words: *Tsunami, Virtual Reality, Disaster Mitigation Education*

Tsunami kill many human beings and damages economic activities seriously, such as tsunami caused by the Great East Japan Earthquake in 2011. It is very important to develop useful modelling, simulation and visualization methods for tsunami waves in order to perform the planning and design for the community development and the prevention of disaster. The visualization is also important to understand the power of tsunami and to improve the consciousness of disaster prevention. Recently, the visualization using the virtual reality (VR) technology is becoming more popular for numerical simulations.

In this presentation, the modelling, simulation and visualization methods are presented for tsunami waves. For the modelling method, several GIS, CAD and AUV data are employed. The stabilized finite element method is employed for tsunami based on the shallow water equation. We also propose a visualization system linked to the evacuation simulation using virtual reality technology to understand the power of tsunami and the importance of the evacuation. The present modelling, simulation and visualization methods are shown to be useful tools for disaster mitigation education.

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Multiple Time Scales and DG Methods for Multi-Layer Ocean Modeling

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Key Words: Ocean modeling, multiple time scales, discontinuous Galerkin

The large-scale dynamics of the ocean contain motions that vary on a wide range of time scales. For the sake of computational efficiency, numerical models of ocean circulation generally split the fast and slow motions into separate subsystems that are solved by different techniques. The fast motions are represented by a vertically-integrated system that is similar to the shallow water equations. The other subsystem employs governing equations in each of the fluid layers. In this situation, it is essential to maintain various kinds of communication and consistency between the two subsystems. This talk will discuss such measures in the case where the spatial discretization is accomplished by discontinuous Galerkin (DG) methods. These measures include some ones that were recently encountered in the context of thin layers that can arise when layer interfaces outcrop to the upper surface of the fluid or when layer interfaces intersect variable topography at the bottom of the fluid.

Multivariate Flood Fragility Analysis for USACE Inland Levees

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Key Words: *fragility analysis, flood prevention, overflow, inland levees*

Floods cause more casualties than any other natural hazard in the United States so flood protection barriers like levees are highly important to preventing devastating damages to life and infrastructure. Levees can be classified according to their risk assessment as with the United States Army Corps of Engineers (USACE) Inland Levee Classification system [1], and according to their composition and structure. Understanding how different classes of levees perform during one of the most common failure events, overflow failure, can help improve flood prevention measures by predicting when, where and how levees will fail. This study serves to analyze the performance of several classes of levees during overflow failure and create flood fragility models to assess their capabilities. The parameters used as random variables for the fragility models are discussed in detail and the results of the study will be reported using graphical and analytical data. Numerical results detailing the conclusions gathered and further research necessary to make this study more robust will be presented.

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On the shallow water, diffusive, and kinematic flow approximations for modeling rainfall runoff

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Key Words: Shallow water flow, diffusive wave equation, kinematic wave equation, rainfall runoff, finite element

Rainfall runoff can be a significant contributing factor to inland flooding during hurricanes due to the accompanying torrential rainfall that often occurs. When the rainfall rate exceeds the local infiltration rate of the inland area, overland flow occurs in the form of rainfall runoff. While this overland flow can be modeled using the full shallow water equations (with the addition of a source term for rainfall), simpler approximations to the shallow water equations — namely, the diffusive and kinematic wave approximations — have been shown to accurately represent overland flow under conditions often encountered in natural watersheds. In this work, we compare numerical solutions to the full shallow water, diffusive, and kinematic wave flow equations for a variety of rainfall runoff flow scenarios and discuss the merits of each approximation in terms of accuracy and computational cost.

Representation of Coastal Protections in the Shallow Water Equations Without CFL Restrictions

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The shallow water equations provide the basic modeling equations for a number of coastal flooding hazards, such as tsunamis and storm surge. In realistic scenarios there are often structures important to these flows that have a large extent but small width, including sea-walls, berms and harbor barriers. Explicit time stepping schemes, most often used for the shallow water equations, can therefore suffer from time step restrictions due to the CFL condition. In this talk, we introduce a set of approaches that sidestep these issues by allowing a barrier to have zero-width and to cut a cell arbitrarily without suffering from CFL restrictions. This is done by supplementing existing Riemann solvers and leveraging cut-cell methods that preserve the properties of the Riemann solver and add negligible cost to the original solvers.

Time Domain Sound Field Analysis Using the Finite Element Method and the Fast Multipole Boundary Element Method

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Key Words: *Finite Element Method, Boundary Element Method, Noise Barrier, Auralization*

Noise is one of the seven major types of pollution in Japan, and it leads to the highest number of complaints according to a survey published by the Ministry of Internal Affairs and Communications in December 2021. Especially in urban areas, the evaluation of noise has been an urgent issue for planning and designing various constructions, such as roads, railways, and airports. Several evaluation methods for traffic noise simulation have been utilized. Based on the frame of reference used, those methods can be classified into two categories: 1) Methods based on the geometrical acoustic theory and 2) Methods based on acoustic wave theory. Both methods have advantages and disadvantages. For geometrical acoustic theory methods, the CPU time is very short but the numerical accuracy is comparatively low. Acoustic wave theory methods, on the other hand, provide accurate solutions but large-scale simulations.

This paper presents a noise evaluation system based on acoustic wave theory. This paper utilizes two methods – the finite element method [1] and the boundary element method using a fast multipole method [2], which are employed for the discretization of unsteady wave equation – and compares the numerical results of the benchmark problem. In addition, we show the results using the analytical model of the complex shape based on standard specifications of noise barriers and discuss the difference of the numerical results and auralization results between the two methods.

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Towards Improved Storm Surge Modelling Using Spaceborne GNSS-R Systems

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Key Words: *Global Navigation Satellite Systems Reflectometry (GNSS-R), tropical cyclones, storm surge, CYGNSS*

The ability to provide accurate meteorological input wind fields is key for accurate storm surge modelling and prediction. Because tropical cyclones spend most of their life cycle in the open ocean and exist over large spatial scales, direct *in-situ* wind observations are challenging. Cyclone winds also can evolve rapidly, particularly as they make landfall. These challenges motivate exploring the use of remote sensing measurements of ocean winds for storm surge prediction. NASA's Cyclone Global Navigation Satellite System (CYGNSS) Earth Venture Mission (EVM) [1]-[2] is particularly well suited for this purpose and for providing insights into storm surge inducing tropical cyclone wind fields and their evolution in time. CYGNSS uses GNSS-Reflectometry in which CYGNSS's eight satellite-based receivers together with GPS satellites form a bistatic radar geometry (the GPS satellites act as transmitters and CYGNSS satellites act as receivers) such that over any given measurement reporting period (typically 0.5-1 seconds), the constellation is capable of providing 32 measurements of ocean winds. These measurement properties allow CYGNSS to provide extensive spatial coverage and frequent temporal revisits when compared to other ocean wind speed remote sensing approaches.

This presentation will present updates on a previously reported 'matched filter' framework in which CYGNSS's 'special-mode' full-DDM measurements are used to estimate maximum tropical cyclone winds that are further used to produce cyclone wind fields using a parametric approach [3]. Particular emphasis is placed on the potential for using CYGNSS's measurements for the accurate retrieval of maximum hurricane winds relative to independent reference datasets. The use of these CYGNSS-derived wind fields in ADvanced CIRCulation (ADCIRC) model storm surge simulations will also be presented, along with a discussion of the utility of spaceborne GNSS-R system measurements in storm surge prediction. Results from the approach are compared with storm surge predictions using 'Best Track' derived wind fields and with available *in situ* storm surge data for storms of interest over the period 2017-2021.

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A general review on microstructural properties of bacteria-based self -healing cementitious composites

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Key Words: *Bacteria, Cementitious Composite, Microstructure*

In order to achieve self-healing ability and to prolong the lifespan of cementitious composites, incorporation of bacteria has been investigated in recent decades [1]. The incorporation of bacteria into cementitious composites has advantages on repairing cracks which cracks can be autonomously and perpetually sealed via calcite precipitation of the bacteria [2]. Moreover, microbial-induced calcite precipitation is reported to densify the microstructure of the cementitious materials, thus can improve mechanical performances including the compressive strength and permeability of the cementitious materials [3]. Carbonate ions released by the ureolytic activity of the bacteria can combine adjacent cations to precipitate carbonate minerals which are able to reduce porosity in the microstructure [2]. Consequently, dense microstructure and enhanced mechanical performances can be achieved by the microbial-induced calcite precipitation. This paper revisits earlier works on the microstructural properties of the bacteria-based cementitious composites. An initial work on the early stage hydration of the bacterial-based cementitious materials will also be briefly presented [4].

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Applicability of Large-Scale Finite Element Analysis to Nonlinear Problems of Concrete Structures

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Key Words: *Large-Scale Analysis, Concrete, Smeared Crack, Boundary Nonlinearity*

This paper presents a study for large-scale nonlinear analysis of civil engineering structures. Conventional structural calculations of civil structures are performed using frame analysis based on beam and spring elements to reduce computation time. However, these simplified numerical modeling approaches are not necessarily required owing to the recent development of computers that enable computing of complex problems. In addition, the numerical modeling must be elaborated for complicated large-scale problems, such as the seismic safety assessment of critical infrastructure (e.g., nuclear power plants) and performance-based design to evaluate the certain performance directly without traditional specifications. In this study, large-scale parallel analysis is employed to improve efficiency when solving the abovementioned problems. The analysis procedure is based on the open-source code FrontISTR[1], deployed using the parallel finite element method (FEM). Furthermore, nonlinearity characterizing the behavior of concrete structures is introduced into the large-scale analysis.

Concrete structures exhibit the combinations of several sources of nonlinearity. In this study, we considered the effects of material nonlinearity and boundary nonlinearity. First, a non-orthogonal multi-directional smeared crack model[2] is implemented to accurately simulate the material nonlinearity of concrete material. This model accepts multiple cracks in an element so that it is appropriate to simulate complicated crack failure under cyclic loading, such as the seismic response. Next, we employed a contact analysis procedure based on penalty method to address the boundary nonlinearity. Therefore, the large-scale nonlinear analysis method of concrete structures is achieved.

Finally, we examined the applicability of the proposed method to large-scale problems through the nonlinear seismic response analysis of a concrete gravity dam and its foundation. The dam is separated into a certain number of cantilever monoliths by contraction joints, so that strong earthquake can induce opening-closing of the joints and crack failure of concrete material. The numerical results revealed that the proposed method can evaluate preceding nonlinear behavior of the dam and the practicality and scalability of the proposed method are sufficient for practical purposes. Therefore, it is concluded that the proposed method can overcome the large-scale nonlinear problem of concrete structures in the future.

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Preliminary Computational Analysis of Structural Performance and Damage of Reinforced Concrete Slabs Subjected to Open Air Blasts

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Key Words: *Reinforced Concrete Slab, Air Blast, TNT, Finite Element Analysis, Concrete Damage*

Explosive loading can be a serious threat to urban buildings and infrastructures [1]. An explosion can be defined as a large-scale and high-speed release of energy, and it generates a huge amount of shock waves. The shock wave can be classified as high explosive when it is faster than the speed of sound and as deflagration when it is slower than the speed of sound [2]. Civil engineering mainly deals with high explosive phenomena that can cause damage to civil infrastructures.

Explosive substances can exist in solid, liquid, or gaseous state, and most of the high explosive phenomena are caused by solid explosive substances such as trinitrotoluene (TNT). In the case of TNT, a typical solid state explosive substance, 3000-4000°C gas is expanded to a pressure of 250-350 tonf/cm^2 when exploding in the air [3]. As a result, the expansion of air generates shock waves, thereby releasing energy to destroy the reinforced-concrete (RC) structures. However, the level of damage of RC structures may vary depending on the arrangement of rebars, concrete properties, and design of the structure.

In the present study, preliminary computational analysis of the structural response and damage of reinforced concrete (RC) slabs subjected to open air blast by using LS-DYNA explicit code. For computational analysis, various TNT mass levels were considered and implemented to ConWep code in LS-DYNA to simulate shock pressures on RC structures. First, incident and reflected pressures were numerically predicted and compared with measured pressure data [4]. Then, rear displacement and damage of RC slabs were computationally predicted and compared with the air blast experimental data [4]. Finally, an applicability of the computational approach using ConWep code in LS-DYNA to the optimal blast protective design will be discussed.

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Recent progress in piezoresistive CNT-incorporated polymeric composite sensors: An overview

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Key Words: *Conductive polymeric composites, Carbon nanotube, Piezoresistive sensor*

In recent years, studies have focused on the utilization of conductive polymeric composites for sensing applications [1,2]. Conductive polymeric composites have been practically applied in many sensing fields such as strain sensors, thermostats, and stretchable transistors [1,2]. Carbon nanotube (CNT) is one of the typical electrically conductive fillers consisting of conductive polymeric composites. Owing to their high aspect ratio and outstanding electrical conductivity, electrical pathways can be readily formed in a polymer matrix with only small amounts of CNTs [1]. Researchers have developed various piezoresistive CNT-incorporated polymeric composite sensors, reporting that the electrical resistance of the composites has been found to increase with increasing strain but remains almost constant as strain is released [2,3]. This paper overviews recent progress in piezoresistive CNT-incorporated polymeric composite sensors, including initial work on micromechanical prediction of the sensors done by the authors [4].

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Reviews on micromechanics-based failure analysis for fiber-reinforced laminates via Puck failure criteria

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Key Words: *Micromechanics, Fiber-reinforced Laminates, Failure Analysis, Damage evolution*

In the past few decades, fiber-reinforced laminates (FRLs) have been widely used in various infrastructures owing to their high strength, durability, and rigidity [1]. Based upon inherent characteristics of FRLs, the presence of some inevitable defects such as micro-crack, void, fiber debonding, and an imperfect interface between fiber and matrix lead to difficulty in the failure analysis [2]. Correspondingly, the inevitable damage parameters of FRLs should be well addressed to precisely predict the failure [2]. Many of the relevant studies have been reported that void growth, fiber debonding, and imperfect interface potentially provoke the inter-fiber fracture (IFF), leading to inevitable damage factors in FRLs [2,3]. For the failure analysis of the IFF, the micromechanical framework considering the micro-void growth and fiber debonding has been proposed [3,4]. Puck failure theory can also be adopted as a phenomenological and physical analytical method to predict the failure analysis in FRLs [4,5]. This paper reviews micromechanics-based failure analysis for FRLs specifically via Puck failure criteria [5]. In addition, a preliminary study conducted by the authors to predict the behavior of the FRLs is briefly introduced [5].

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Utilization of coal bottom ash for the alkali-activator in geopolymer composite

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Key Words: *Bottom ash; Geopolymer; alkali activation; strength; expansion;*

This research investigates a new method for application of bottom ash in geopolymer composite. Bottom ash is a by-product of thermal power plants, and many studies have been conducted to utilize bottom ash for geopolymer. However, it is difficult to use a large amount of bottom ash due to reasons such as decrease in strength, gas generation, and expansion. Therefore, in this study, a method of using bottom ash as an activator was developed. The degree of activation of bottom ash was analysed through ICP and pH test. Also geopolymer composites were conducted compressive strength and expansion test. It was observed that a large amount of gas was generated and escaped in the process of dissolving the bottom ash in the activator, and the compressive strength was also increased compared to typical method of replacement. Based on the result, it is expected that the suggested method of utilizing bottom ash can be an effective solution to consume large quantities of bottom ash in the concrete industry.

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Axial compressive response of circular tubes with lattice core fabricated by powder-bed fusion process of metal 3D printer

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Key Words: Circular Tubes, Lattice Core. Axial Compression, FEM, Energy Absorption

Thin-walled circular and square tubes have been widely used in automobiles, ships and aerospace engineering as main structural parts owing to their effective energy absorption capacity per unit mass. There are many studies concerning the static and dynamic response of thin-walled tubes under axial compression[1, 2]. One of our co-authors has also published a paper regarding the estimation technique of the initial peak load for circular tubes subjected to axial impact loading[2].

Recently, more and more attention have been paid to improve the energy absorption capacity of tubes by adding porous materials such as foams and honeycomb cores in the tubes[3]. On the other hand. due to the novel development of additive manufacturing technology, a precise and complex lattice cores with the length of micrometres can be fabricated easily, and their stiffness and strength have been investigated by many researchers.

In this paper, the axial compressive response of lattice-cored sandwich tubes has been studied by using a nonlinear finite element method. The effects of micro-architecture of the lattice core and the overall geometries of the sandwich tube have been investigated. In addition, the lattice-cored tubes were manufactured by using our in-house metal 3D printer, and their axial compression tests have been conducted. The numerical and experimental results agree well with each other, and their great abilities of the energy absorption by the existence of lattice core have been confirmed.

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Creasing Instability Analysis Focusing on Energy Barrier and Energy Bottom

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Key Words: *Creasing, Energy barrier, Energy bottom, Finite element analysis*

In this study, we investigate the creasing instability using a perturbation force-based analysis and clarify the energy barrier necessary for the occurrence of the crease and the stable state of the crease, named energy bottom. Two-dimensional finite element analysis is conducted on the elastomer assigned with the incompressible Neo-Hookean material, along with considering compressive strain and wavelength of the crease as parameters. A perturbation force is applied to a point on the top surface of the elastomer. To simulate the creasing, we introduce the artificial viscosity, and later its effect is removed.

When a perturbation force works enough to get over the energy barrier, the crease is induced on the top surface of the elastomer. The energy barrier becomes smaller with increasing strain. In addition, the high resolution of finite elements makes the energy barrier small. These tendencies have already been reported in the previous study [1]. On the other hand, the energy barrier is independent of the wavelength of the crease. Thus, the onset of creasing is not affected by the scale of deformation.

Once the stored energy gets over the energy barrier, the crease quickly grows toward the energy bottom. The energy bottom is independent of the mesh resolution, unlike the energy barrier, which means that the evolution of the crease can be reasonably simulated. The wavelength of the crease at the energy bottom increases with a rise in applied compressive strain [2]. On the other hand, as applied compressive strain approaches the threshold of creasing, the wavelength converges to a specific length.

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Experiments and Simulation of Ductile Fracture Considering Damage History for High-Strength Steel Sheets

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Key Words: *Pressure effect, Lode dependence, Finite element analysis, Digital image correlation*

Over the decades, the ductile fracture behaviours of metals have been studied by many researchers [1]-[4]. In the classical metal plasticity, it is assumed that the hydrostatic pressure has negligible effect on the materials strain hardening, and that the flow stress including the initiation of fracture is independent of the third deviatoric stress invariant. However, recent experiments on metals have shown that the both the pressure effect and the effect of the third deviatoric stress invariant should be included in the constitutive description of the materials [1]-[4].
In this study, the relationship between stress triaxiality and fracture strain of high-strength steel sheets that are widely used for many parts in automobiles was investigated through the nonlinear finite element analysis (FEA) and the strain measurement using stereo digital image correlation (Stereo-DIC). In the experiment, tensile load was applied to a notched thin sheet specimen, and the displacement and strain distributions on the both surfaces of a specimen were measured using a dual Stereo-DIC system. Then, not only the time-variation of the in-plane strains but the through-thickness strain and the stress triaxiality during the test were evaluated. In this numerical study, damage growth was considered in our FE model with a customized subroutine program. The results show that the relationship between the stress state of the high-strength steel sheet and fracture strain can be predicted with high accuracy by comparing with the experimental results. It was found that the larger the stress triaxiality, the greater the effect of damage.

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Finite element analysis of fracture strength in ceramics based on the Generalized Pareto model for pore size distribution

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Key Words: *FEM, Damage model, Fracture mechanics, Grain size, GP model, Extreme value statistics*

Structural ceramics have excellent properties such as heat resistance. However, the problem is that there is a large variation in strength compared to other materials. This is due to the distribution of microscopic defects inside the ceramics [1]. In order to reproduce these characteristics, the author's group has proposed a finite element analysis method to predict the variation in fracture strength of ceramics based on internal microstructure data (relative density, pore size distribution, grain size distribution, etc.) [2][3]. However, there is still room for improvement in this approach. One of them is that the analysis results depend on the mesh size.

In this study, we aimed to improve this problem by applying the Generalized Pareto (GP) model, one of the extreme value statistics, to the pore size distribution. The pore size distribution is the most important factor in the fracture strength of ceramics among the internal microstructure data. AS999, a high-purity alumina (Al_2O_3), is used as the target material, and data on the size and number of pores are measured by X-ray CT. Then, the parameters of the GP model were determined using the PWM method. Furthermore, the threshold of minimum pore size was determined to 0.009 mm based on the mean excess plot.

In the finite element analysis, pores is generated randomly in each element while according to GP model, and the maximum value among them is adopted as the maximum pore size in respective elements. It should be noted that the number of generated pore is adjusted to the change in mesh size.

As a result, our method was able to reproduce the results of the three-point and four-point bending tests, including the scatter of strength. The same three-point bending test was also performed with different mesh sizes of the specimens, and the test results were also reproduced.

In summary, this study was able to solve the mesh size dependency, which was an issue of the previous method [2][3]. In addition, in the process of applying the GP model, we developed the general scheme to determine the internal structure data from the measurement results by X-ray CT. In the future, we will study how to apply the measurement results by SEM and other methods.

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Incremental Mean-Dilatation Method for Coupled Thermo-Mechanical Problems in Nearly Incompressible Solids

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Key Words: *Nearly incompressible, Thermo-mechanics, Incremental variational formulation*

In this study, we propose an incremental mean-dilatation method to conduct thermo-mechanically coupled analysis on nearly incompressible materials. To this end, we define the thermo-mechanically coupled energy rate potential in line with an incremental variational framework (IVF)[1]. The energy rate potential contains three kinds of energy potential, internal energy, dissipation potential, and Fourier potential, and also considered the incompressible condition with Lagrange multiplier[2]. Then, the equilibrium temperature stemming from the volume change is originally introduced in connection with the introductions of volume change and pressure, which are constant in a whole domain of continuum body.

As a result, the established thermo-mechanically coupled problem, including control of volume change, is variationally consistent, so that we can enjoy several benefits associated with numerical accuracy and efficiency. For example, taking advantage of the benefit, which the consistent tangent modulus necessarily becomes symmetry, the fully implicit update algorithm based on the standard type of Newton-Raphson method can be constructed. Further, the proposed method can avoid the volume locking occurring in the use of the lower-order element, which is expected to improve the computational stability and efficiency.

To validate the applicability of the proposed method in practical use, the several numerical problems for hyperelastic and standard dissipative solids are solved by means of three kinds of numerical methods: standard IVF with 1st order element, standard IVF with 2nd order element, the proposed method with 1st order element.

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Numerical study on effect of boundary condition for collapse behavior of plate subjected to axial compression and bending

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Key Words: *FEM, Plate, Compression, Bending, Buckling*

In this research, the collapse behavior of a thin plate subjected to axial compression and bending is studied by using the finite element method. For various boundary conditions, the stress distributions at ultimate are compared with international specifications. The collapse of the plate which has various hardening characteristics is investigated. It means that local buckling, post-local buckling redistribution of stress and critical strain are investigated. Based on the above investigation, an approximate prediction of the collapse stress was proposed. Further, its validity was verified comparing with the numerical results by the FEM under various material and geometric properties.

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Progressive Collapse Analysis of Heavily Loaded Pallet Rack Systems Subjected under Impact Loads

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Key Words: *Pallet Rack System, Progressive Collapse, Impact, ASI-Gauss Code, FEM*

Pallet rack systems used in warehouse are generally constructed with light weight uprights and beams, and are frequently subjected to accidental impact by forklift trucks [1]. When heavily loaded, those impact may cause partial or progressive collapse of rack systems which will mostly lead to catastrophic loss of goods and sometimes of human lives [2].

In this study, numerical investigation was conducted on progressive collapse behavior of rack systems using the Adaptively Shifted Integration (ASI) - Gauss code [3], which can supply highly accurate elasto-plastic solutions with minimum subdivision of finite elements and can stably simulate nonlinear phenomena such as member fracture and contact. Push-down and push-over analyses with and without upright removal were carried out on a two-bay rack system to observe the standard strength and effects of plan bracings installed at different levels. Furthermore, dynamic analyses with impact load in cross-aisle and down-aisle directions under fully- and over-loaded conditions were conducted and the effects of plan bracings were investigated.

According to the numerical results, plan bracings installed at first level affect greatly against lateral impact at lower levels, and those installed at top level affect greatly in preventing downward collapse making the most of its catenary action. Progressive collapse analysis of a large-scale pallet rack system was also conducted and the effect of optimal installation of plan bracings was confirmed.

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Study on Thin Reinforced Concrete Slabs Subjected to low-velocity Impact - Preventing scattering debris by using steel deck plates -

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Key Words: *Steel Deck, Steel Pipe, Reinforced Concrete Slab, Impact Test, Finite element analysis*

When constructing a building above public traffic lines such as roads and railway tracks, it is necessary to ensure sufficient safety to the space under the slabs. If a hanged object fall and perforate the reinforced concrete slab, and debris caused by the impact are scattered under the slab, those could cause serious consequences such as human casualties. This study focuses on those debris scattering under the slab. To prevent this, this study proposes an anchoring mechanism into concrete at the edge of steel deck plate used as permanent formwork.

In a typical steel-framed building, slab is constructed by pouring concrete on the deck used as a permanent formwork. Since the deck is usually not anchored into the concrete, it can easily fall off by the impact, and the generated debris scatter under the slab. In this study, the deck is anchored into the concrete by folding up the deck plate ends. The anchoring mechanism would be effective in preventing the deck plate from falling off by the impact, and damaged concrete from scattering.

In this study, half scale impact tests were conducted on specimens assumed to be RC slabs used in buildings, and it was confirmed that the proposed anchoring mechanism was effective in preventing the deck plate from falling off and scattering debris. In the cases without the anchor mechanism, the deck plate fell off at a falling height of 7.5 m, but in the case with the anchor mechanism, the deck did not fall off at 14 m, and fell off at 15m.

Moreover, it was confirmed that the effects of this experiment behaviour could be evaluated by finite element analysis. This analysis was performed with LS-DYNA. The anchoring mechanism between the concrete and the deck plate was reproduced using tie-break contact in LS-DYNA. In the case with the mechanism, the deck falling off and debris scattering were suppressed at a falling height of 13m in the analysis as well as the test. In addition, the falling object velocity, penetration depth of impact area of the slab, and reaction force were also in close agreement with the experiment.

It is now possible to suppress the scattering of debris caused by the impact under the slab in the event of a collision with a falling object during construction work above the public traffic line, thereby improving the safety of the lower part of the slab. As a result, such construction work can be made smoother, which will contribute to the advanced use of space on public traffic lines and the development of the city.

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3D Slope Stability Analysis Considering Influence of Infiltration and Surface Flow

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Key Words: Green-Ampt Infiltration, Surface Flow, Hovland Method, 3D Slope Stability Analysis

Because landslides caused by heavy rainfall have occurred every year all over the world, landslide mitigation and prevention are recognized as a global issue. Although a lot of slope stability analyses[1] have been reported, it is still difficult to predict landslide occurrence in a wide area with time-series data of rainfall. To overcome this problem, this study presents a novel framework for rainfall-induced landslide prediction by combining hydrodynamics and three-dimensional slope stability analysis.

In the proposed framework, infiltration analysis using the Green-Ampt model and two-dimensional surface flow analysis are employed to represent water transportation induced by rainfall. Regarding to the three-dimensional slope stability analysis, the Hovland method is employed on the assumption of ellipsoid-shaped slip surfaces. The infiltration depth at each calculation point is evaluated by the infiltration analysis and surface flow analysis, and the obtained spatial distribution of infiltration depth is used as an input datum for the slope stability analysis. A part of the area in Kamaishi City, Iwate Prefecture, located in the northeast of Japan, is selected as a target area for analysis. A lot of landslides occurred in the target area due to a typhoon attacked on October 12 and 13, 2019. Detailed terrain data measured using UAV were obtained before and after the typhoon. In addition, the actual slope failure locations were identified through a field survey. These data are used to verify the accuracy of the numerical analysis. The obtained results indicate that the proposed framework has a high potential for the predicting rainfall-induced landslides. It should be also noted that the results manifest that small forestry roads affected landslide occurrence.

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A Numerical Study of the Bulk Viscosity in the Cumulant Lattice Boltzmann Method on Tsunami Impact Pressure

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Key Words: Lattice Boltzmann method, Cumulants, Free-surface flow, Volume-of-fluid, Bulk viscosity

Free-surface flow problems occur in numerous disaster simulations such as tsunami in an urban area. The characteristics of these flow fields are three-dimensional, highly non-linear and non-hydrostatic. A fully three-dimensional free-surface fluid model is required to simulate such a flow field. In recent years, the cumulant lattice Boltzmann method (CLBM) [1] has attracted much attention as a novel simulation method and has been successfully applied to various engineering fields.

In CLBM, the bulk viscosity is set independently of the kinematic viscosity. It is one of the critical parameters determining the accuracy and stability of impact pressure estimation in the weakly compressible flow model. When the bulk viscosity is set appropriately, the acoustic error caused by excessive numerical oscillations due to sound waves can be suppressed. However, if the bulk viscosity is too large, the calculation accuracy may be degraded. To ensure accurate calculations while suppressing the numerical oscillation of the pressure, the bulk viscosity must be validated.

In this study, we proposed a single-phase free-surface flow model based on CLBM using the volume-of-fluid (VOF) model to capture the interface. We performed the dam-breaking flow problem [2] to validate CLBM for estimating impact pressure in the violent flow field. The relationship between the bulk viscosity and impact pressure was examined. We demonstrated that values of the bulk viscosity between 0.6 and 1.0 are reasonable in terms of the reproducibility of peak pressure and suppression of pressure oscillations for violent flow fields. The results of the proposed model are in good agreement with the experimental results. It is concluded that the free-surface flow model using CLBM is an advantageous method for calculating the impact pressure acting on a structure, which suppresses the numerical oscillation.

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Clarification of the Damage Mechanism of the Long-Period Bridge System Damaged by the 2016 Kumamoto Earthquake

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Key Words: *Long-Period Bridge System, 3D FE Model, 2016 Kumamoto Earthquake*

The purpose of this study is to clarify the damage mechanism of a long-period bridge structure-underground interconnected system, such as the Ohkirihata Bridge damaged in the 2016 Kumamoto earthquake, subjected to the combined loads of long-period pulsive ground motions, surface fault displacements, and ground deformation by slope failures.
Firstly, the site-specific waveforms were estimated by the finite difference method as input ground accelerations to a bridge system model. Secondly, the target bridge system was modeled by three dimensional (3D) finite element (FE) method with 441,196 nodes and 2,437,126 solid elements. The target bridge system is the affected Ohkirihata Bridge which is a 5-span continuous steel girder bridge with the length of 265.4 m long and the width of 12.5 m wide. For the 3D FE model, the reinforced concrete (RC) slabs and steel girders were idealised by equivalent tetrahedral first-order elements with Young's modulus and density of mass of parallel serises of slabs and girders. The five laminated rubber bearings with total rubber thickness of 85 mm -150 mm are placed upon the top of each pier: A1Bs, P1Bs-P4Bs, A2Bs. The layers of natural rubbers and steel plates consisting of a bearing were modeled by hexahedral first-order elements with same plain size and different heights. The RC piers P1-P4 and RC abutments A1, A2 were modeled by tetrahedral first-order elements. The RC foundations of caisson piles supporting P1, P4 and A2 and cast-in-place piles supporting A1, P2 and P3 were modeled by tetrahedral first-order elements. The underground layers consist of nine different soil materials which mechanical properties were identified by soil tests. These shallowed layers were modeled by tetrahedral first-order elements. The minimum sizes of all tetrahedral first-order elements were set as about 1m in average. The stress-strain relationships set for all elements were assumed to behave isotropically in the elastic ranges.
We used a open-source program for large-scale parallel computation of FE analysis: FrontISTR. Linear dynamic analysis was performed by applying the site-specific waveforms of the main ground motions for 10 seconds as equivalent inertial forces to all nodes of the 3D FE model. The Newmark-β method (β=0.25, γ=0.5) was used in the time integration scheme. The time interval was set to be 0.005 sec, and the number of computational steps was 2000. Damping effect on equations of motion was formulated by stiffness-proportional damping matrix. The CG method was applied for the numerical linearization, and the SSOR preprocessing was used. The threshold for determining the convergence about relative error of computed displacement was set at 1.0×10^{-6}.
P3B, P2B, P4B, A2B, and P1B, in that transient order, exceed allowable shear strain of 250% in the 3.9 seconds before the maximum amplitudes of the site-specific EW and NS waveforms, and A1B follows to exceed 250% after the peak. The time-series horizontal motions of the superstructure supported by these bearings until the 3.9 seconds are demonstrated as first, the superstructure moves to the northwest direction between 1.86 s and 2.49 s, next to the southeast direction between 2.49 s and 2.82 s with a slight clockwise rotation around the A1, and further to the north direction between 2.82 s and 3.24 s with a counterclockwise rotation around the A1. The reasons are why the excitation of long-period pulsive ground motions to the primary eigenmode of the target bridge system in the 1.2 s to 1.5 s natural period causes these processes.

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Hybrid seepage failure analysis between two-phase mixture flow techniques using an ISPH-DEM coupling method

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Key Words: ISPH-DEM, Resolved and Unresolved coupling, Karman vortex

As global warming progresses and seismic activity increases, landslides caused by torrential rains and tsunamis by huge earthquakes are becoming more frequent. There is no end to the damage to structures and human lives continue to occur all over the world. To estimate the damage level of these natural disasters in advance, numerical simulations using the particle method, which can predict the post-collapse behaviors, have been considered promising.

We develop a fluid-soil coupling analysis solver using ISPH [1] and DEM, which are both Lagrangian particle simulators, to analyze the seepage failure of a breakwater mound caused by a tsunami [2]. Since the simulator is suitable for reproducing discrete phenomena such as slope failure with sediment separation and merge, it can also estimate the protection effects of the breakwater with permeable gabions. Resolved coupling technique without permeability is applied to the caisson blocks and un-resolved coupling technique, which treats as a macroscopic seepage flow analysis, is applied to the soil mound and the gabions modeled by DEM. The coupling simulator reproduces the seepage failure process including the overturning and sliding of caissons and the backward erosion of mounds.

On the other hand, quantitative evaluation of the seepage failure of the rubble mound, in which the un-resolved coupling technique is applied, is a difficult issue because it relies on an empirical macroscopic drag force model. Through numerical tests, we recognize a hybrid technique between the resolved and un-resolved model may become more effective for the two-phase mixture flow of soil and water. Before the development of hybrid techniques, we have been working on the improvement of ISPH fluid analysis (negative pressure calculation, gradient, and Laplacian model, etc.) to reproduce the pore flow in the pore space between soil particles in detail by micro-scale Resolved coupling analysis. Then, we simulate the Karman vortex street behind the cylinder and sphere in the flow channel using these methods.

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Improvement of a tsunami scenario detection framework by using synthetic geodetic data

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Key Words: *Tsunami scenario detection, synthetic GNSS data, POD, Bayesian update*

Tsunamis are one of the most significant coastal risks in the international community. Especially in Japan, which is frequently threatened by earthquakes and its subsequent tsunami inundation, considerable attention has been paid to the expected Nankai-Trough earthquake and tsunami in the next few decades, which will be an event with extremely short evacuation time (<30 mins) for the residents. Although there have been many tsunami forecast systems proposed, there is still room to improve minimizing the uncertainties relevant to the deterministic numerical simulations or erroneous/noisy data acquired in real-time.

This study focuses on the improvements of the previous tsunami scenario detection method [1], which uses a form of unsupervised learning and sequential probability updates. We now also incorporate geodetic data measured at GNSS stations. The fakequakes software [5] is used to generate 600 synthetic kinematic slip distributions for Nankai-trough-going ruptures, based on techniques developed in [2,6], along with the corresponding seafloor deformations and synthetic GNSS waveforms. The subsequent tsunami propagation and inundation in Kochi city, which is located in southern Japan, are realized by GeoClaw [3]. Then the approach developed in [1], which utilizes both POD and a Bayesian update, is used to identify the most similar tsunami scenario from a pre-computed database, which is a priori tagged together with its geodetic information. The validity of the predicted tsunami scenario is evaluated by either the wave history data at some synthetic gauges offshore, or the maximum inundation values in coastal zones. The previous reports on the use of GNSS data to improve tsunami forecasts [4] are examined in the context of our approach, by testing the combined/solitary use of GNSS (and the synthetic wave history data at gauge points).

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Numerical Study on Damage of Tsunami Evacuation Building under Tidal Wave and Debris Impact

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Key Words: *Tsunami evacuation building, Debris impact, Fluid-structure interaction, Partitioned FSI analysis, Particle method, ASI-Gauss method, Improved ERP model*

Robustness of a tsunami evacuation building is one of the most important problems in protecting lives and properties against tsunami. To ensure robustness, it is necessary to design with consideration of strict external forces, including dynamic fluid force and debris impact force, caused by tsunami.

In this research, we numerically simulate behaviour of a tsunami evacuation building under tidal wave and debris impact to investigate trend of the forces due to tsunami. Partitioned fluid-structure interaction analysis scheme coupled with stabilized ISPH (Incompressible Smoothed Particle Hydrodynamics) method [1] and ASI (Adaptive Shifted Integration)-Gauss method [2] is applied for the simulation. The ISPH method is a semi-implicit particle method and suitable for free surface flow problem such as tsunami. The ASI-Gauss method is a finite element method using linear Timoshenko beam elements and can express a plastic hinge at any position in an element by shifting a numerical integration point. Besides, improved ERP (Explicitly Represented Polygon) wall boundary model is used as interface modelling between fluid and structure domain. This model accurately satisfies boundary conditions on solid walls and can directly calculate fluid force exerted on the walls.

As validation of the proposed FSI coupling scheme, we solved free fall problem of a beam member and dam break problem with an elastic obstacle. Results of these analysis showed that the coupling scheme can obtain precise solution. Furthermore, we conducted a simulation of a tsunami evacuation building under tsunami and debris. Specification of the building was determined according to current tsunami evacuation building design standard in Japan [3]. Based on the results, damage of the building caused by tidal wave and debris impact was verified.

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Optimization of offshore gauge configuration for early tsunami forecast with GA and POD

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Key Words: *Early tsunami forecast, Genetic algorithm, Bayesian theory, Gauge placement optimization*

Large earthquakes and the subsequent tsunamis cause extensive damage to coastal areas as experienced in the 2011 Great East Japan Earthquake. In recent years, people are concerned with the Nankai megathrust earthquakes in Japan, and the coastal area of Shikoku, which is close to the plate boundary, is expected to be attacked by a tsunami immediately after the earthquake. Thus, an early tsunami forecast is extremely important for evacuation and damage mitigation. For early and reliable tsunami forecasts, a lot of cable networking systems (e.g., S-net, DONET) have been installed in the ocean surrounding Japan. However, such multiple ocean gauges should be reasonably placed realizing the early forecast under limited resources.

In this study, we propose an optimization framework to identify effective placement of gauges for the early tsunami forecast, based on the recently developed scheme[1]. Our optimization framework employs the Genetic Algorithm(GA) for detecting the placement of n gauges from $N(\gg n)$ candidate gauges, based on the data extracted from the Proper Orthogonal Decomposition(POD). Thanks to the POD technique, we can carry out GA-based optimization with the dimensionality reduced data, which allows us to handle it more efficiently. According to the previously developed scheme, we calculated the tsunami propagation by TUNAMI-N2[2] for the 1564 earthquake scenarios from Mw 7.6 to 8.8 occurring in the Nankai Trough. Then the wave height data at $N = 131$ candidate gauges are stored for each simulation result. With the characteristics of the spatial wave height distribution and the scenario-specific information, which are both extracted from POD, we could determine the n=10 sensitive gauges for the tsunami prediction by applying GA. As a validation, the scenario-specific information of a test scenario extracted from the $n = 10$ observation gauges is compared with all stored scenarios. The likelihood calculated from the sequential Bayesian updates is then used to forecast the incoming tsunami wave by weighted average. Our gauge placement optimization further sophisticates the recent early tsunami forecast system, which has advantages because they only require the likelihood calculation of the scenario using the wave height observations, without time and cost-consuming numerical simulations. Although the tsunami forecast demonstration focuses on the Nankai megaquake and the Shikoku coastal area, our framework can be applied to other earthquake scenarios and regions.

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Real-time tsunami forecast by combined use of Bayesian updates and POD - A case study in Westport (Washington) -

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Key Words: *Tsunami mitigation, Early forecast, POD (Proper Orthogonal Decomposition), Bayesian Update*

The coast of North America located near the Cascadia subduction zone is known to be exposed to a huge earthquake/tsunami risk, although there was little awareness of this until the second part of the 20th century. The papers [1] and [2], for example, suggest that the subduction zone caused at least 18 major earthquakes in the last 10,000 years. Since the last significant earthquake occurred more than 300 years ago, the necessity of earthquakes and tsunami mitigation along the North-West coast of America seems imperative in the recent century. In this study, we evaluate the risk of tsunami triggered by earthquakes in the city of Westport (Washington) by applying the method proposed in the previous study [3] which combines Bayesian update and Proper Orthogonal Decomposition (POD). The results are compared to other data [4].
The plausible earthquakes at the targeting sites were generated by a fakequakes (fake earthquakes) software [5], and a tsunami database has been created with GeoClaw [6] considering 4 magnitude classes: M7.5, M8.0, M8.5 and M.9.0. In total, 1964 earthquake/tsunami scenarios have been created and wave history data at 30 gauge-stations were stored for the forecast process. The concept of our forecast scheme is to determine the closest scenario from the scenario database to the occurring tsunami by comparing their main characteristics, i.e. the characteristics of their time-histories. Such characteristics are extracted by POD which enables reducing the computation cost and time of the process. Then, by using the Bayesian update, uncertainties are minimised at each time step. During the whole process, particular attention is paid to the observation-time required to obtain the closest scenario to the occurring tsunami and to the evolution of the closest scenarios themselves. The forecast process is fast as the database has already been studied before the occurrence of the event and at a low cost as the main characteristics only are compared. We could also consider combining a few of the most similar scenarios. The measures of the new event are made in the shortest time period possible.

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Research on Tsunami Evacuation Simulation Considering Population Change and Snow Cover Conditions

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Key Words: Tsunami, Evacuation, Great East Japan Earthquake, Multi-agent simulation

In the Tohoku region, a large tsunami is expected to occur in the near future, due to the occurrence of earthquakes with epicenters along the Japan Trench[1]. In addition, there are declining birthrate and aging population, and it is necessary to keep the population age distribution in mind when considering future tsunami disaster prevention.
In this study, we focused on Yamada Town, Iwate Prefecture, which was severely damaged by the Great East Japan Earthquake, and analyzed its residents' evacuation. performed by a multi-agent system NetLogo, adopting evacuation behavior in the previous research[2], and using open data on future population[3]. The population numbers in 2020 and 2045 were set as the initial evacuee population, three cases of the evacuation start time (10, 15, and 20 minutes after the earthquake) were set. In addition, in consideration of the decrease in evacuation speed due to snow accumulation on the road in winter, and analysis was performed when evacuation was performed at low speed.
As a result, that compared to the case where evacuated 10 minutes after the earthquake, for those who evacuated 20 minutes later, the rate of non-arrival at the evacuation center would increase by about 20 points. Furthermore, it was found that when the evacuation speed in winter was applied, the rate of non-arrival at the evacuation center was higher than in summer. In the future, it is considered necessary to proceed with the evacuation verification analysis in consideration and respond to people requiring assistance during a disaster due to the declining birthrate and aging population.

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Tsunami Forecasting from Sparse Observations by Semi-Supervised Outlier Detection with Generative Adversarial Network

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Key Words: *Tsunami Forecasting, Generative Adversarial Networks, Outlier detection*

A tsunami warning should be issued quickly using limited observational data. Liu et al. [1] construct regression models of tsunami amplitudes at locations in the Salish Sea based on hypothetical sea surface elevation observations near the entrance of the Strait of Juan de Fuca: a support vector machine was used to predict the maximum amplitude at the forecast points, two convolutional neural networks (a denoising autoencoder and a variational autoencoder) to predict the full-time series at the forecast points. Herein, we transform the regression problem of tsunami amplitude into a binary classification problem with high waves as positive examples and others as negative examples. The transformed problem can be considered as a supervised outlier detection problem since large Tsunamis are rare events. To extract the effective feature from a small number of high waves, we consider applying semi-supervised outlier detection methods. In Shimauchi [2], it was shown that the augmentation of the extracted representations by unsupervised learning methods using a generative adversarial network (GAN) enhances the performance of supervised outlier detection on several datasets.

Liu et al. [1] used a set of 1,300 synthetic data of megathrust earthquake on the Cascadia Subduction Zone, which was generated by Melgar et al. 2016. Gauge 702 (located near the entrance of the Strait) is considered as an observation point. Forecast points are assumed as Gauge 901 (located deep in Discovery Bay where fieldwork has uncovered tsunami deposits) and Gauge 911 (located in the middle of Admiralty Inlet). We set thresholds (3 meters and 5 meters) for the Gauge 901 and Gauge 911 in the data: the data points that exceed the thresholds are labelled as positive and other data as negative. The percentage of positive examples is 5% to 26%. The labelled data is split into training sets and testing sets. The baseline model of the experiment is a classification model by a support vector machine.

In the experiment, we used ROC-AUC (the area under the receiver operating characteristic curve) and precision@n (the true positive rate for the top n results in a dataset that contains n outliers) on the testing datasets as evaluation metrics. The average and standard deviation of each metrics in ten independent trials were used in the evaluation. The method in Shimauchi [2] achieved the best scores in all cases: precision@n, ROC-AUC are 81-85%, 0.97-0.99. In particular, precision@n and ROC-AUC are improved 6-18%, 3-5 compared to the baseline. The standard deviation is also improved except in one case. The experiment may suggest that accurate Tsunami forecasting is possible by semi-supervised outlier detection with unsupervised representation learning and GAN even when the observation data of Tsunami is small, under certain settings.

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A Duality-based Coupling of Cosserat Crystal Plasticity and Phase Field Theories for Modeling Grain Refinement

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Key Words: *crystal plasticity, Cosserat continuum, phase field, dual problem, grain boundary, reproducing kernel approximation*

High-rate deformation processes of metals entail intense grain refinement and special attention needs to be paid to capture the evolution of microstructure. In this work, a new formulation for coupling Cosserat crystal plasticity and phase field is developed [1]. A common approach is to penalize kinematic incompatibility between lattice orientation and displacement-based elastic rotation [2]. However, this can lead to significant solution sensitivity to the penalty parameter, resulting in low accuracy and convergence rates. To address these issues, a duality-based formulation is developed which directly imposes the rotational kinematic compatibility. A weak inf-sup-based skew-symmetric stress projection is introduced to suppress instabilities present in the dual formulation. An additional least squares stabilization is introduced to suppress the spurious lattice rotation with a suitable parameter range derived analytically and validated numerically. The required high-order continuity is attained by the reproducing kernel approximation. It is observed that equal order displacement-rotation-phase field approximations are stable, which allows efficient employment of the same set of shape functions for all independent variables. The proposed formulation is shown to yield superior accuracy and convergence with marginal parameter sensitivity compared to the penalty-based approach and successfully captures the dominant rotational recrystallization mechanism including block dislocation structures and grain boundary migration.

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A General Terrain-Fitted Coordinate System for Modelling Hazardous Shallow Flows in Mountain Area

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Key Words: *Hazardous shallow flows; Terrain-fitted coordinate system; Cartesian Coordinate system; Digital elevation map (DEM); Mountain area*

It is non-trivial to model the hazardous shallow flows in Mountain area. It is fraught with complexities of two kinds: on the physical side, various constitutive relations are requested and have to be postulated due to the complex composition. On the modelling side, depth-integration is often employ for reducing the complexity of computation over a large domain. The Cartesian coordinate system, with *xy*-plane lies horizontally and *z*-axis pointing upwards vertically, is generally adopted for its ease of describing the constitutive relations and rugged topography. However, the depth-integration process may yield high deviation of velocity direction in case the topographic surface does not tangential to the horizon, because the flow follows on the basal surface. In the terrain-following coordinate system, the depth-averaged velocities are tangential to the basal surface, so that it can fix this drawback of velocity direction deviation. But the terrain-following coordinate system is generally limited by the constrain of shallow curvature for the topographic surface, especially when obstacles (e.g. sabo dam) are constructed in the flow paths.

In the present study we propose a general approach, which integrates the terrain-following coordinate and conventional Cartesian coordinate systems. For highly rugged topography, the terrain-fitted coordinate axes are assigned to coincide with the Gaussian-filter-smoothed basal surface, on which the highly rugged landform sits (called “sub-topography”). In comparison with the conventional Cartesian coordinate, this approach reduces the deviation of the flow velocity deviations, and the constraint of shallow curvature is fulfilled without losing the precision of the landform. It is interesting to find that the coordinate axes tend to be straight and are comparable to the Cartesian ones after Gaussian filtering for infinite times. In other words, it is a general approach of unifying the terrain-fitted coordinate system and the Cartesian coordinate one.

Numerical examples are employed with respect to a two-phase grain-fluid model (Tai, et al., 2019) for investigating the results computed based on the Cartesian approach and on the one with sub-topography in terrain-fitted coordinate system. All the computations are performed by a CUDA-GPU accelerated simulation tool, MoSES_2PDF (Ko et al., 2021). And a back-calculation of historical event (2009 Hsaiolin landslide event) will be shown for highlighting the potential of engineering application.

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Deep Learning Enhanced Dynamic Meshfree Analysis

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Key Words: *Meshfree Method, Dynamic Analysis, Recurrent Convolutional Neural Network, Surrogate Model, Computational Efficiency*

Dynamic meshfree analysis requires the computation of structural response recursively at each time step, which significantly increases the computation burden since in each time step, the complexity in meshfree approximation already introduces high computational cost. In this work, the intrinsic relationships are established between the meshfree discrete data and the machine learning training samples, and between the recursive computational procedure of dynamic meshfree analysis and the temporal sequence information transmission mode of recurrent convolution neural networks. Meanwhile, it is also shown that there is a strong similarity between the receptive fields of convolutional neural network and meshfree supports.

With the aid of these intrinsic links, a recurrent convolutional neural network structure design method for meshfree discretization is proposed, which is then used to develop a recurrent convolution neural network surrogate model for dynamic meshfree analysis. This surrogate model takes full advantage of the flexibility of meshfree discretization. Meanwhile, meshfree analysis can provide versatile and highly accurate numerical samples, which then enhance the generality and applicability of the proposed surrogate model for dynamic meshfree analysis. In addition, the unique historical memory characteristics of the recurrent module embedded in the recurrent convolution neural network surrogate model enable an effective processing of the sequence information, and then accelerate the dynamic meshfree computation. The efficiency and accuracy of the proposed method is demonstrated through several examples, including large deformation meshfree modelling of slope failure.

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Development of Numerical Simulation on Inland Water Flooding Using Local Inertial Equations

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Key Words: *Inland water flooding, Local inertial Equations, DEM*

This study aims to develop a numerical simulation model for inland water flooding. Recently, extreme weather conditions have increased short-time heavy rains in Japan, so inland water flooding occurs frequently. Therefore, an accurate prediction of flooding in real-time is required. However, few studies have been conducted to shorten the calculating time while enhancing analysis accuracy. In this study, we develop a high-accurate simulation of inland water flooding based on local inertial equations. The local inertial equations are suitable for relatively slow currents. We performed the simulation of the steady flow and the overflow on a weir and obtained effective calculation results. Furthermore, the numerical model was applied to downtown Morioka city in Iwate Prefecture, and the characteristics of inland water flooding in the area were cleared.

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Eulerian-based Finite Element Simulation of Landslide-induced Consequences on Submarine Infrastructure

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Key Words: *Submarine Landslides, Shear Bands, Impact Force, Eulerian Formulation*

Submarine landslides are the underlying cause of some of the most devastating natural disasters. They may cause the disappearance of entire regions along the shoreline, generate tsunami waves, and destroy the offshore infrastructure. The already existing and future planned gas transportation infrastructure along the continental slopes requires a better understanding of the processes that result in subsea landslides in order to improve our ability to predict, assess, and mitigate their potential hazards.

Unfortunately, laboratory and field studies cannot reproduce realistic subaqueous landslides. Computer simulations, on the other hand, enable us to simulate full-scale events and specific set-ups that are impossible to build in the laboratory (e.g., limiting material properties, extreme velocities, or large dimensions). Moreover, computer simulations usually cost much less than laboratory experiments, and they can reproduce much more complex and versatile phenomena. While some essential field data may be missing or impossible to collect, by changing possible geometric conditions (e.g., bathymetry, potential weak zones) and soil mechanical properties, it is possible to assess the upper and the lower limits of potential consequences of the landslide and possible hazards to subsea infrastructure. Moreover, through parameter analysis, it is possible to define how important each missing parameter is.

The process of landslide evolution involves large deformations and movements of the soil. In such problems, the traditional Lagrangian finite element approach, typically implemented for problems in soil mechanics, suffers from excessive element distortions and, therefore, cannot be adopted to analyze the above phenomenon. In the present work, the computational framework adopts an Eulerian approach [1-2]. In the Eulerian approach, the material is free to move through the mesh, which is fixed in space. Consequently, the problem of excessive element distortions becomes irrelevant. Several advanced continuum approaches to treat large deformation problems in soil mechanics exist; however, the main advantage of the Eulerian framework is that it is widely available within commercial codes, such as Abaqus, Ansys, LS-Dyna, etc., accessible to engineers. Moreover, Abaqus software, for example, can easily adapt various enhancements and modifications employing user subroutines and Python codes.

We demonstrate the framework through several examples of landslide events, including the impact on offshore infrastructure. The importance of the landslide trigger mechanisms is underlined.

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Extraction of Disaster Area from Satellite Image by combining Machine Learning and Image Processing Technology

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Key Words: *Satellite Image, Machine Learning, Land Cover Classification, Additive Color Mixture*

In recent years, heavy rain which frequently occurs in various parts of Japan causes severe damages. It is important to identify the damaged area for disaster recovery and reconstruction.

To identify the damaged areas, a number of research have been conducted using satellite images. However, most the research has used the synthetic aperture radar (SAR) which is complicated to process, and the research using the optical satellite images has been limited to the preliminary level.

Therefore, in this study, we focus on the optical satellite images that are easy to process and interpret, and extract the damaged area by combining existing methods such as a land cover classification method by machine learning and an additive color mixing method.

With regard to the extraction of the damaged areas, it is necessary to extract the land cover changes. Therefore, we prepared the images before and after the disaster. First, we performed the land cover classification on the pre-disaster images and post-one. The results of the land cover classification showed that the land objects in the satellite images were properly classified. However, it was found that it was difficult to properly classify land objects below the resolution of satellite images (e.g., two-lane roads). Next, we applied an additive mixture method to extract the changes in land use before and after the disaster. As a result, it was found that the number of pixels indicating buildings decreased, while the number of pixels indicating fields increased in the damaged areas. It can be said that the area indicates the damaged area.

Based on the above results, it is possible to visually express the land cover changes before and after the disaster in a specific categories and to extract the damaged area.

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Numerical Modeling of Phase Transformation Induced Material Fracture and Crack Propagation

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Key Words: *Phase transformation, Fracture, Mesoscale model, Crack propagation*

The physical mechanisms triggering intermediate-depth earthquakes remain a puzzle for the scientific community. However, many studies discussed phase transformation being the primary mechanism behind the generation of these hazardous earthquakes. The objective of this study is to develop a numerical model for the simulation of phase transformation-induced failure in geo-materials. The materials of interest include different groups of minerals found in the earth crust such as granulite, eclogite, and olivine. To model the phase transformation behavior, a thermo-mechanical model approach has been taken. A thermodynamically consistent multiscale model, based on Mahnken et al, 2015, has been developed to capture the evolution of phase transformation taking place in such materials under different pressure and temperature conditions. In the model, each material point of the macroscale consists of polycrystals at the mesoscale level. Further, each crystal on the mesoscale is composed of various phases or variants of phases on the microscopic level. Crystal structure of different phases or variants has been incorporated through the rotated transformation strain in the model where additive decomposition of total strain has been used. The model is also capable of including different material properties for different phases or variants of phases and captures the orientation effect by including different orientations of grains at the mesoscopic level. The model also considers visco-plasticity and heat conduction and uses a volume averaging scheme to link different length scales. In the numerical scheme, the solution of coupled non-linear equations for the evolution of visco-plasticity and phase transformation has been obtained by a staggered algorithm. Implementation of the abovementioned thermomechanical model has been done using a user subroutine in a commercial finite element software ABAQUS. Validation of the model has been done using data for phase transformation from austenite to bainite and for olivine to spinel. For the simulation of microstructural failure in the material, the extended finite element method has been used with the above-mentioned model. A Higher amount of crack propagation has been observed from preliminary results of the model with phase transformation as compared to the case without any phase transformation under the same loading and boundary conditions. The effect of temperature has also been studied on the phase transformation and crack propagation for the olivine to spinel transformation. The model will be further validated with the data obtained from the laboratory experiments done on the materials of interest to investigate the phase transformation-induced instability leading to the formation of macrocracks. For further study, the model will eventually be upscaled to simulate the fault generation at the macroscale (kilometer-scale) and investigate the role of phase transformation in the formation of large-scale cracks or faults.

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Effect of particle distribution and clustering degree of cement particles on the hydration process using a numerical approach

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Key Words: *Reconstruction, Microstructure, Cluster, Simulation, Cement Hydration*

Microstructural characteristics of cementitious materials are crucial in determining the mechanical properties of the materials. For a better understanding of the behavior of cementitious materials, microstructural characterization and reconstruction methods, coupled with modeling and simulation, have been issued in the field of computational modeling of cement paste. For instance, microstructural imaging techniques such as a scanning electron microscope (SEM) image and its probabilistic description have been widely used to generate multi-phase microstructure. However, because of the complexity and limitations of the current approaches, it is highly desirable to develop a new method to model cement particles effectively.

This study aims to propose a model for generating virtual pre-hydrated specimens of cement paste using only very limited information, such as chemical composition and particle size distribution. In particular, the influences of the particle distribution and clustering degree of cement particles on the hydration process were investigated using computational simulation. For this purpose, the cement particles with different sizes were modeled based on the experimental data, and phase clustering of the main components, such as C_3S, C_2S, C_3A, and C_4AF, was controlled according to the chemical composition and quantitative information of several types of cement. Using the probabilistic description methods, the degree of phase clustering can be adjusted, and the virtual pre-hydrated cement microstructures with different phase distributions can be generated. The results of hydration for 28 days of each microstructure were obtained from a numerical approach using CEMHYD3D and then compared with the experimental data of a target cement.

The obtained results confirmed that the virtual specimen with a large degree of clustering shows a similar hydration profile to the experimental results. In particular, a significant difference in heat of hydration occurred during the initial reaction within a few minutes, which can affect the mechanical properties of cement paste. This indicates that the investigation of microstructural characteristics during the hydration process according to the degree of clustering can provide insights for a better understanding of multi-phase cement-based materials.

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Image based connected aggregate segmentation of concrete using complementarity of X-ray and neutron tomography

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Key Words: *Concrete microstructure reconstruction, aggregate segmentation, X-ray tomography, Neutron Tomography*

For the realistic microstructure representation of concrete, connected aggregate segmentation is performed using the 3D CT images obtained from the complementarity of X-ray and neutron tomography. For the aggregate segmentation, most available techniques either reduces the aggregate volume fraction by eroding its surface area or over segment the aggregates particles which leads to inaccuracy of their size distribution. In this study, a recursive surface erosion and reconstruction algorithm was used to segment connected aggregates particles without having the previous issues [2]. As a result, disconnected aggregates can be classified according to their size and reconstructed in 3D in order to validate the accuracy of the presented technique. Additionally, characterization of the segmented aggregates such as their diameter, area, volume and circularity/roundness distribution was performed. The characteristics are compared in 2D and 3D before and after segmentation. Image analysis results show the advantage of the 3D segmentation and the good agreement between the images analysis and concrete mixing design.

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Image based data-driven approach for material property prediction

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Key Words: Convolutional Neural Network, Microstructure, Property, Cement Paste, Micro-CT

The uncertainties of microstructural features affect properties of materials. The distribution characteristics of pores in cementitious material have great influence on its mechanical properties, and numerous pores that are randomly distributed in the material make it difficult to predict the material's properties. Existing studies are limited to the analysis of the statistical relationship between pore distribution characteristics and material responses [1], and the correlation between them is not yet fully determined. In this study, the mechanical response of cementitious materials is predicted through an image-based data approach using convolutional neural network (CNN), and the correlation of pore distribution and material response is analyzed.

The dataset for machine learning consists of high-resolution micro-CT images and properties (stiffness and strength) of cementitious materials. The microstructures are characterized, and the mechanical properties are evaluated through 2D direct tension simulations using the phase field fracture model [2]. Algorithms are developed to predict the material response when micro-CT images are inserted into input-data of CNN. Since the material responses need to be calculated for machine learning, various algorithms are used to prevent overfitting even for small size datasets. In the model with high learning accuracy, attribution of input image is analyzed [3] to identify the spot in the sample with the greatest influence on the prediction of material response. This study analyzed the correlation between pore distribution characteristics and material response by comparing the active region during the CNN process and the pore distribution.

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Measuring material nonlinearity of concrete using nonlinear Rayleigh surface waves

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Key Words: *Non-destructive Evaluation, Nonlinear Ultrasound, Rayleigh Surface waves, Microcracks*

In this paper, the nonlinear elastic behavior of cement-based materials under various kinds of damage is monitored using nonlinear Rayleigh surface waves. During several decades, numerous researchers have paid much attention to nonlinear ultrasonic techniques including nonlinear resonant ultrasound (NRUS), nonlinear wave modulation (NWMS), nonlinear wave mixing, and second harmonic generation (SHG) to characterize early-stage damage state in solid materials [1]. Among them, SHG using nonlinear Rayleigh surface waves holds a great promise for in situ assessment of full-scale concrete structures because of the advantages in measuring damage parameter regardless of the boundary condition and geometry of target structures. This talk will demonstrate the sensitivity of acoustic nonlinearity parameter, β (i.e., damage parameter) from the SHG method to early-stage microcracking formation in concrete. In comparison with the conventional contact-based detection methods, the robustness of non-contact, air-couple detection technique in precise detection of β is also examined [2]. Then, a variety of physical/chemical phenomena in concrete structures such as the sequestration of carbon dioxide into concrete cover [3], load-induced damage [4], and drying shrinkage [5] is assessed by a measure of β particularly with an emphasis on monitoring microcracking development. Finally, some synergetic effect of the proposed method towards improving infrastructure maintenance is discussed.

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Microstructural characteristics of cement mortar using cockle shell aggregates and waste fishing net fibers

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Key Words: *Cement Mortar, Microstructure, Cockle Shell, Waste Fishing Net*

According to the development of ostreaculture, numerous marine products are consumed in South Korea, and related waste becomes a serious problem simultaneously. To overcome the problems caused by marine wastes, recycling or utilizing marine produces becomes an issue in many engineering fields. In the construction material industry, several researchers have used waste materials as supplementary materials and demonstrated that proper use of marine products can be an effective approach to recycle the waste. Moreover, the use of recycled supplementary materials needs to be considered for the development of eco-friendly construction materials.

This study aims to investigate the effect of cockle shells as an aggregate replacement on cement-based materials. For this purpose, a series of cement mortar specimens were produced, and the crushed cockle shells were used as a substitute for fine aggregates. In addition, ground waste fishing nets were utilized as a fiber replacement to enhance the flexural performance of cementitious materials. Both cockle shells and waste fishing nets were washed with an ultrasonic cleaner in order to remove the influence from foreign substances or salt damage and ground accordingly considering the sizes of fine aggregates and polypropylene fibers. The cockle shell and the waste fishing net were then used as substantial materials for fine aggregates and fibers, respectively. 10, 20, and 30 wt.-% of cockle shells were substituted for fine aggregates, and the waste fishing net of 0.5, 1.0, and 1.5 % of the total volume was also considered in the mixtures. The compressive and flexural strength of the specimens were measured to examine the effect of replacement on the mechanical properties. Scanning electron microscope (SEM), X-ray diffraction (XRD), and micro-computed tomography (micro-CT) were utilized to investigate the microstructural characteristics of the materials with different substitution ratios.

The obtained results confirm that a proper substitute of fine aggregates with cockle shell powder can be used as alternative materials for conventional cement mortar, and the waste fishing net can be also utilized as a reinforcement for the flexural performance of cementitious materials.

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Microstructural Characterization of Fiber−Matrix Interface and its Mechanical Property Evaluation

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Key Words: PVA Fiber Reinforced Cementitious Compsites, Microstructure, Fiber-Matrix Interface

The cementitious material is widely used in construction, but it has low tensile strength and displays brittle failure. To overcome such disadvantages of cementitious materials, the polyvinyl alcohol (PVA) - fiber reinforced cementitious composites (PVA-FRCCs) is developed [1]. Owing to its high strength and large elastic modulus of PVA fibers, PVA-FRCCs exhibit multiple cracking and strain-hardening behaviors. However, the fiber-matrix interface affects mechanical responses significantly, and it is important to characterize the fiber-matrix interface, and to evaluate its mechanical properties.

To characterize the fiber-matrix interface, 3D microstructures obtained from micro-CT images are investigated. In addition, field emission scanning electron microscope (FE-SEM) images are acquired to observe 2D microstructures of fiber-matrix interface in high resolution. A new segmentation method is proposed to characterize the fiber-matrix interface from micro-CT images effectively, and the 3D microstructures of PVA-FRCCs are successfully segmented into 3 phases (i.e., pore, PVA fiber, solid). The mean solid linear attenuation coefficient ($\bar{X}_{solid}$), and porosity are used as characterization parameters [2]. Using the 3D microstructures characterized by the micro-CT, simulations are performed to evaluate the effects of fiber-matrix interfaces on the mechanical behaviors of PVA-FRCCs. The proposed framework is expected to provide insights on the microstructural behaviors of complex materials by synergistically combining the state-of-the-art approaches of the experiments and simulations.

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Monitoring the Effect of Cellulose Microfibers on Internal Curing of Cement Composites Using Linear and Nonlinear Resonance Techniques

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Key Words: *Internal curing, cellulose microfibers, nonlinear resonance, linear resonance, and crack density*

While the use of cellulose microfibers in cementitious materials has increased as a means of facilitating internal curing at early-age, issues associated with their interaction with cement matrices, the formation of microstructure, strength, etc., have not been fully understood. Utilizing linear and nonlinear acoustic techniques can be a promising approach because of the ability to detect both early-stage damage originated at microscale or mesoscale cracks. This talk will present a procedure for linear impact resonance acoustic spectroscopy (LINAS) and nonlinear impact resonance acoustic spectroscopy (NIRAS). Specifically, a hysteretic and nonlinear elastic behavior of cellulose microfibers-reinforced cement composites is assessed via the nonlinearity parameter, α. Together with the measurements of longitudinal wave velocity, the resonance frequency is also measured to estimate the crack density. Then, petrographic analysis and porosimetry confirm the presence of water desorption by cellulose microfibers and provides the evidence of internal curing. The results show that the measured α from the NIRAS test is sensitive to the microstructural change in cement composites, revealing the effect of cellulose microfibers on the internal curing, while the resonance frequency is capable of detecting the mesoscale change, showing a strong correlation with the measured crack density. Finally, the results highlight the potentials for this approach with an emphasis on carbon neutralized cementitious materials.

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Prediction of Mechanical Response for Heterogeneous Materials considering Spatial Phase Distribution

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Key Words: *Heterogeneous material, Microstructure, Phase field fracture model, Micro-CT, Nanoindentation*

Cement paste is one of the typical heterogeneous materials in the construction field, which has a complex microstructure with several phases. The behaviours of the cement paste are significantly affected by the spatial distribution of its components. To predict its mechanical response, it is necessary to investigate the phase distribution characteristics and identify each phase properties. Therefore, a framework to evaluate the mechanical properties of the material with complex microstructure based on characteristics of each phase through combining experiment and simulation is introduced in this study.

A virtual specimen of a microstructure for cement paste is constructed from micro-CT images. It can be segmented into several phases, such as pore, hydration products, and anhydrous cement; the linear attenuation coefficient value [1] of the micro-CT images is used as the phase characteristics. The virtual specimen reflects actual distributions of the phases, so that the complex behaviour of crack propagation can be detected from a simulation using the phase field fracture model [2]. Modeling input parameters of each phase for the simulation are obtained from nanoindentation test. The effect of considering multiple phases on the material response is investigated through a comparison of the behaviour between homogenized single and multiple phase solid models. The proposed framework can provide the guideline to design the new cementitious materials according to the purpose, and this study can be used for material property prediction of various heterogeneous materials.

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15th World Congress on Computational Mechanics (WCCM-XV)
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Two-scale Analysis of Mechanical Properties for Cement Paste by Synergistically Combining Experimental and Computational Approaches

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Key Words: Phase Field Fracture, Microstructure, Property, Cement Paste, micro-CT, Multiscale Analysis

Microstructures of cementitious materials are complex, and it is not trivial to effectively evaluate and predict their properties. To develop innovative cementitious materials for sustainable and safe infrastructures efficiently, accelerated tools combining experimental and computational approaches are required. In this study, a synergistic tool for identifying mechanical properties of cementitious materials is presented through a two-scale (micro-macro) analysis framework.

At the micro-scale, microstructures of a cement paste are obtained from a high-resolution synchrotron micro-CT. The microstructures are characterized, and the mechanical properties are evaluated through direct tension simulations using the phase field fracture model [1] with the input paramters determined from nano-indentation test results. The homogenized properties are then linked to the upper-scale (macro-scale) microstructures, which are also obtained from a synchrotron micro-CT. At the macro-scale, in-situ micro-CT tensile splitting tests measurements are conducted. The experimental results are compared with the computational results, where the homogenized input parameters were homogenized from the micro-scale analysis. The multi-scale framework is expected to provide insights into the accelerated development of the innovative cementitious materials.

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Combination of physics-based and data-driven modeling for nonlinear structural seismic response prediction

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Key Words: Deep Neural Network, Residual Network, Explicit Integration, Augmented State

Despite great progress in seeking accurate numerical approximator to nonlinear structural seismic response prediction using deep learning approaches, tedious training process and large volume of structural response data under earthquakes for training and validation are often prohibitively accessible. In our methodology, the main innovation can be seen in of integration of deep neural networks (DNN) with a classical numerical integration method by using a hybridized integration time-stepper. In particular, we set the nonlinear restoring force vector as augmented states, and hence change the original nonlinear differential equation into a linear one, so that common explicit integration algorithms in control theory for linear time-invariant dynamic system can be applied. We propose to use residual network (ResNet) to learn time-stepping schemes specifically for the nonlinear state variables of the system. The original explicit integrator is then supplemented with the the DNN time-stepper with dimensional expanding. Our DNN-Augmented (DNN-A) time-stepping scheme provides important advantages over current pure data-driven approaches, including (i) a flexible framework incorporating known time-invariant physics information, (ii) requirement of structural seismic response data being circumvented by simple short bursts of trajectories collected from underlying nonlinear components, and (iii) efficiency in training and validation process. It is also remarkable that the proposed approach is parallelizable and allows relatively large time-steps. Several numerical examples are presented to demonstrate the performance of the methods.

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Comparison of Analysis Results between Two Analysis Programs by Parametric Study of Thousands of 3D Building Structure Models

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Key Words: *3D building structure model, parametric study, seismic response analysis,*

With the development of computers in recent years, 3D analysis of building components has begun to be used for seismic response analysis of buildings. The demand for seismic response analysis using 3D building structure models is increasing in order to understand the behavior and safety of large buildings by evaluating the nonlinear characteristics of members caused by long-period earthquakes. The FEM programs used in conventional building structural design perform the analysis using the static implicit method. Since the static implicit method requires the solution of multiple simultaneous linear equations, the calculation time for large-scale buildings is often large. Therefore, reducing the time for seismic response analysis in 3D building structures models is an important issue in implementing large-scale projects. On the other hand, general-purpose detailed FEM programs use the dynamic explicit method to perform the analysis. Since the dynamic explicit method does not require the solution of simultaneous equations, the computation time tends to be smaller than that of the static implicit method. It is important for designers who use these programs to conduct parametric studies to understand the differences in analysis time, memory usage, stress and deformation behavior between them. However, it is not easy to perform a parametric study on a large scale 3D building structure models by manual operation.

The purpose of this report is to conduct an automated parametric study of several thousand 3D building structure models and to collect the results of seismic response analysis by two programs, in order to prepare for analysis of the differences between the results of the two programs.

We investigated the analysis time of a large 3D building structure model using implicit and dynamic explicit seismic response analysis software. As a result of the analysis on a Windows desktop PC, it was confirmed that the analysis time was reduced by 92% when the dynamic explicit method was used rather than the implicit method. In order to understand the modeling methods and material properties of members in the two programs and to compensate for the differences between them, a material property test of a simple one-member model was conducted. As a result of the material property test, it was confirmed that it is necessary to input parameters to take into account the movement hardening because an arbitrary plastic rotation angle-bending moment relationship defined using a load curve shows isotropic hardening behavior as a skeleton curve. In order to investigate the results of the implicit and explicit methods on a large scale 3D building structure model, we developed a program to automatically generate parameters for parametric studies using thousands of 3D building structure models.

In the future, the results of parametric studies using thousands of 3D building structure models will be statistically processed to analyze the results of the implicit and the explicit analysis. Then, we aim to improve the speed in seismic response analysis of 3D building structure models.

Damage Recognition of Wooden House Using Deep Neural Network Trained with Simulated Responses Considering Epistemic Uncertainty

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Key Words: *Wooden Building, Epistemic Uncertainty, Deep Neural Network, Structural Health Monitoring*

The Data Science Working Group of the Numerical Shaking Table Committee of the National Research Institute for Earth Science and Disaster Resilience is working on the development of structural health monitoring technology using artificial intelligence.

In the 2016 Kumamoto earthquakes, some residents returned to their wooden houses that had been severely damaged by the strong ground motion, and the houses collapsed due to the following main shock causing human casualties. This kind of disaster should be reduced if they could understand the remaining performance of the house using a structural health monitoring system.

Deep neural networks have been reported to achieve high accuracy in various fields in pattern recognition and evaluation of regression equations with a large amount of training data. The authors have also taken the same approach of preparing big data for training by conducting time history response analysis with many input earthquake motions and damage patterns in advance [1], [2].

However, the stiffness and strength of the members assumed at the design stage do not necessarily match the actual values of the completed building. Epistemic uncertainty exists, and it is desirable to recognize damage patterns and evaluate residual performance with features that are robust to such variations.

In this study, we propose a method of generating training data with variability based on the results of elemental experiments conducted in conjunction with full-scale wooden building experiments in the E-Defense experiment, and constructing training data by providing input seismic motions of appropriate intensity so that the number of training data with and without damage is balanced.

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Data Assimilation Using the Quality Engineering for the Seismic Response Analysis of 3-Story Wooden Houses

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Key Words: *Data Assimilation, Quality Engineering, Seismic Response Analysis*

INTRODUCTION

Since the Great Hanshin-Awaji Earthquake in Japan, many full-scale shaking table experiments have been conducted for the purpose of understanding the seismic performance of wooden houses. Then, the knowledge obtained in the experiment needs to be fed back to the simulation such as structural analysis. Compared to the shaking table experiment, the simulation has the advantage of being less costly and time-consuming and being able to visualize and analyse the results when the structure is changed in various ways. However, as a premise that makes them possible, it is indispensable to be able to perform reproducible analysis, that is, "data assimilation: combination of test and simulation". Therefore, in this study, we will examine the method of "data assimilation" for seismic design of wooden houses. In addition, in order to verify its effectiveness, we performed data assimilation for actual table shaking table experiments targeting three-story wooden houses and verified whether it could be reproduced in experiments on different wooden buildings and seismic waves.

RESERCH METHOD

"Data assimilation" is a method that has been developed in the field of meteorological forecasting and forecasting and has been studied as a theory that statistically corrects uncertain factors (initial conditions, model parameters, etc.) of numerical models by observed values. It is useful for improving the accuracy of weather forecasts. On the other hand, "data assimilation" in the field of manufacturing such as wooden construction, spacecraft, and automobiles has been done manually by the intuition and experience of the designer, and it is not only laborious but also dangerous to fall into a special solution. Therefore, from 2020, Kyoto University will focus on the quality engineering, which has the feature that comprehensive search can be performed with a small number of experiments, in joint research with Osaka Institute of Technology and JAXA, and a new target for wooden construction. We are researching various data assimilation methods.

In this study, we defined parameter values such as spring rigidity and yield strength that modelled each seismic element such as joints and walls of a three-story wooden house, and changed them variously by design of experiments. We searched for a combination of input parameters that can be reproduced with high accuracy. It was confirmed that the obtained results can be reproduced with different test specimens and seismic waves. Details and analysis of the results will be described in this conference.

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Dynamic Characteristics Identification of Exposed Column Bases of Steel Building Structures Modeled by Solid Finite Elements

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Key Words: *Dynamic characteristics identification, non-linear structure, exposed column base, solid element*

In this study, it is discussed how to identify the natural frequency of a steel building frame which has an exposed column base and is modeled by solid finite elements. Bending moment-rotational angle relationship of the exposed column base exhibits non-linearity[1], because the steel base plate just comes into contact with foundation concrete and can separate from it due to bending moment. Eigenvalue analyses of vibration are generally conducted to investigate dynamic characteristics of numerical models. In eigenvalue analysis, however, above mentioned non-linearity cannot be considered. In the field of building and civil engineering structures, some materials and structures, such as masonry structures, cables, membranes and so on, show this kind of non-linearity which depends on amplitude and direction of loading.

Here, an exposed column base and first story column are extracted from a three-story steel frame specimen for a full-scale shake table test[2], which was conducted at E-Defense, NIED, Japan. Other parts of the frame are simplified as a rotational spring and a nodal mass at the top of the column. The exposed column base, which consists of components such as a column, base plate, anchor bolts, nuts, anchor plates and foundation concrete, is discretized with solid finite elements and contact, friction, and tying conditions are taken into account in the interface between the components[3]. Then we conduct dynamic analyses of the structure subjected to random ground motions and impulse loadings. The loading level is parametrically varied. By analyzing response displacement at the top of the column, the natural frequency of the target structure is identified and the obtained frequency is compared with the value measured in the experiment.

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Evaluation of the Elastoplastic Behavior of Structures for use as Hysteretic dampers

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Key Words: *Metallic yielding dampers, seismic protection, finite element analysis*

In this research, we proposed 11 hysteretic dampers subjected to shear stresses, with constant height and volume of material to compare their hysteretical behavior. The geometries are based on plate and lattice structures, which are used in energy absorption applications [1].

For the finite element analysis in the software ANSYS, the material failure is modeled using the "ekill" command, which removes the elements that have reached a certain limit value. For validating the material plasticity, boundary conditions, and failure mode, the HHSD damper [2] was replicated, showing a good correlation between our methodology and the experimental results exposed in [2].

The finite element analysis gives the failure modes and the hysteresis curves of the dampers. From this curve, we obtained the elastic stiffness, yield force, yield displacement, ductility, and the number of cycles that the damper supports before decreasing its dissipation capacity. In addition, the graphs effective stiffness vs displacement, effective damping vs displacement, and accumulated dissipated energy vs accumulated displacement were determined for the dampers with equal or better performance than the HHSD since these graphs represent the behavior of a hysteretic damper [3].

From this study it is concluded that the elastoplastic behavior of the hysteretic damper is related to the orientation of the material, therefore it is possible to obtain a better device while maintaining the amount of material if it is oriented correctly. By orienting the material out of the plane, the stresses are better distributed, and greater displacements can be applied to the damper, so lattices structures, in this first study, would be a good option.

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Finite Element Analyses of Four-story RC Structures with Solid Elements and Validation of Results Using Measurement Data Obtained by Full-scale Shaking Table Experiments

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Key Words: *Finite Element Method, E-FrontISTR, E-Defence, RC Structure, Validation*

Earthquakes that exceed the current design criteria of buildings have been occurring frequently in Japan. In order to prepare for the occurrence of unexpected earthquakes, it is important to understand the damage caused to buildings by seismic motion through detailed analysis.

In this study, dynamic seismic response analyses of a four-story RC building are conducted considering the elasto-plasticity of materials, and the numerical results are compared and validated with the results of an experiment conducted at a 3-D full-scale seismic testing facility (E-Defense)[1]. Based on the comparison results, the building model is modified and the effect of the modification is confirmed. In addition, we conduct a data analysis of the analysis results using a large number of measurement data[2]. E-FrontISTR is used for dynamic analyses. E-FrontISTR is a nonlinear structural analysis software developed by Six organizations including the author's research group (NIED, JAMSTEC, CRIEPI, TEPSCO, TAISEI CORPORATION, and ARK Information Systems, INC.), based on FrontISTR[3].

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Global Sensitivity Analysis of Wooden Building Based on Polynomial Chaos Expansion Considering Uncertainty in Material Property

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Key Words: *Structural Health Monitoring, Polynomial Chaos Expansion, Global Sensitivity Analysis, Uncertainty Quantification, Wooden Building*

Structural health monitoring (SHM) is useful for quick and efficient damage recognition of a building under seismic excitation. It has the potential to replace the emergency safety evaluation, which is conducted after major earthquakes in purpose to prevent a secondary disaster from aftershocks. SHM systems are popular for large-scale civil structures in the world, but their application to low-rise buildings such as wooden houses are still limited.

One of the challenges in predicting the response of a wooden structure is that the effect of variance in its material property is considerably significant. To solve this problem, we propose a method using global sensitivity analysis with Sobol' indices based on polynomial chaos expansion (PCE) to find dependent parameters. By considering only material parameters with a high impact on the variability of the quality of interest, we can reduce computational cost in time history response analyses. PCE is a popular technique in the field of uncertainty quantification, which enables us to model the response of a dynamical system with uncertainty. PCE is also known to be highly compatible with global sensitivity analysis, which allows to identify the dependent input variables that contribute most to the variability of the computational model response.

Based on the results of a full-scale three-story wooden building experiments and its member experiments conducted by E-Defense of National Research Institute for Earth Science and Disaster Resilience[1], [2], we performed three-dimensional structural response analyses of a model of the specimen using a numerical collapsing simulation program, wallstat[3]. As input ground motions, we used design ground motion specified by the Building Standard Law with an amplification factor of 120%. Multiple models were prepared with a varied value of material properties to consider the epistemic uncertainty. As a result, the sensitivity analysis clarified that the variance of Young's modulus in columns and beams had a major contribution to the variance of the maximum inter-story drift angle of the model.

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Prototype of Digital Twin Composed of Heterogeneous Seismic Response Simulations in the Urban Cyber Physical System

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Key Words: *Cyber-Physical System, Geographic Information System, Seismic Response Analysis*

We have been developing an urban cyber physical system (CPS) for enhancing resilience against large-scale earthquakes [1]. Concept of the urban CPS is outlined below. Firstly, in the physical space, citizens, enterprises and governments build consensus on desirable state of the city and its evaluation indicators such as gross domestic product, population and quality of life. Secondly, in the cyber space, digital twins predict the state change caused by earthquake disaster, and then find required capacity such as robustness and resilience to satisfy desirable state after the seismic event. Finally, earthquake disaster-prevention technologies are implemented in the physical space to realize the required capacity.

In the digital twin, change in the evaluation indicators caused by earthquake disaster are introduced by predicting and evaluating the state change based on numerical simulations and data analyses. From the gap between the current and desirable states, it suggests optimal countermeasures to realize the desirable state. As to seismic response analyses in the digital twin, flexible selection of different types of simulation technologies are required according to available building information in the city and computational resources.

In this study, we constructed prototype of digital twin composed of heterogeneous seismic response simulations in Masiki, Kumamoto. In this prototype, Integrated Earthquake Simulator (IES) is employed for simplified model of many buildings in the city, wallstat is employed for detailed models of wooden buildings and E-Simulator is employed for a detailed model of an RC building. Building information, damage record in 2016 Kumamoto earthquake and simulation results are visualized on GIS. This prototype system was published on the website [2].

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Slope Disaster Risk Evaluation in the 2018 Hokkaido Eastern Iburi Earthquake using DIPM and GIS

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Key Words: *Depth Integrated Particle Method, Slope Failure, Shallow Landslide, Hokkaido Eastern Iburi Earthquake*

DIPM (depth-integrated particle method) is an efficient numerical method appropriate for sediment-related disaster simulation like slope failure and subsequent long-distance debris flow or mudflow or the entire geo-hazard evaluation of a very wide area with detailed topographic information. The model deals with the flowing mass as a combination of soil columns. Equations of motion of such soil columns are solved as two-dimensional discrete 'particles' moving along the surface terrain. The particles are subjected to bottom shear stress of the flow based on the empirical Manning's formula with yield stress and particle-wise interaction formulated on their hydraulic gradient. Accordingly, the material parameters governing the flow behaviour are only two: the Manning's coefficient, n, and the critical deposition angle, i_{cr} related to the yield stress. The 2018 Hokkaido Eastern Iburi Earthquake triggered thousands of slope failures over a wide area and caused significant losses. Enormous destruction due to multiple slope failures occurred in the towns of Atsuma the north of the epicentre. Two landslides in Yoshino village in Atsuma town were studied for flow simulation. The landslides were shallow and classified as transitional earth slide types. The topographic information was extracted using ArcGIS software from widely available national data such as administrative area, Digital Elevation Model (DEM). From the detailed landslide inventory map available at the Geospatial Information Authority of Japan and flow simulation was conducted by setting the initial slope failure zones and the most appropriate values for n and i_{cr} were identified as 0.10 to 0.15 and 2° to 5° respectively. To select the best-suited parameters, visual and statistical comparisons of the simulation results were conducted. The average accuracy of the simulations was 75%. Slope distribution of the study area was analysed using ArcGIS, and slope stability was calculated using the 1-D slope formula with other researchers' test results from existing field studies. Finally, prediction of slope failure and possible affected areas were generated by the flow simulation for the risk assessment of the selected study area.

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Study on Seismic Response Analysis of a Base-Isolated Building Supported by High Damping Laminated Rubber Bearings Considering Structure-Heat Coupling

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Key Words: *High Damping Rubber Bearing, Base Isolated Building, Structure-Heat Coupling, Finite Element Method, Seismic Response Analysis*

The authors[1] developed a framework for coupled structural and heat conduction finite element analysis for laminated high damping rubber bearings (HDRBs). The coupled analyses were conducted for full-scale tests of an HDRB subjected to several kinds of cycling loading. In the present study, a seismic response analysis of a ten-story RC building supported by two HDRBs is conducted. The finite element mesh used in this study was made in the previous study by the authors[2] for seismic response analyses of the building supported by natural rubber bearings, and the analysis condition is modified to include a constitutive model of high damping rubber.

Damping behavior of an HDRB is due to dissipated inelastic strain energy. The temperature rise is also caused by the dissipation energy. The equivalent stiffness and the equivalent damping factor for an HDRB decreases due to the temperature rise. The influence of the temperature rise on the mechanical properties of an HDRB is smaller than that of a lead bearing. However, the temperature rise in an HDRB subjected to an excitation of an earthquake with long duration and long natural period such as the expected Nankai Trough earthquakes is estimated as 70 to 80ºC. In this case the influence of temperature rise is significant.

The high damping rubber is modeled by an overlaid viscohyperelastic and elastic-plastic constitutive model. In the present study, cyclic coupon tests are conducted for a high damping rubber and material parameters of the overlaid model are identified using the results of the coupon tests. Then, a preliminary seismic response analysis using the analysis model of the base-isolated building considering structure-heat coupling is performed, and the influence of temperature rise on the responses of the building and the HDRBs is investigated.

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Thermo-mechanical Analysis of Reinfoced Concrete Under Extreme Temperature to Assess the Fire Safety of Structures

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Key Words: Thermal cracking, Convective and radiative cooling, Higher order particle discretization scheme, fire safety

Fire incidents post 1995 Great Hanshin and 1994 Northridge earthquake have caused damages to buildings and life-line structures. Despiste adequate seismic performance, reinforced concrete (RC) structures are vulnerable to high-temperature heat as concrete tends to crack under heat and leads to failire of structures. Also, scrapping of megastructures using LASER is an enviorment friendly choice. Therefore, it is essential to have a good understanding of thermo-mechanical response of RC under extreme temperature.

This article presents the formulation and implementation of thermal-shrinkage-induced-cracking to in brittle materials. Convective and radiative cooling, coupled with deformation and cracking, are rigorously treated, and related modules are implemented into a high-order particle-discretization finite element method [1].

Developed modules are verified by comparing with analytical solutions of static and transient heat problems. Modules are further validated by comparing with observations from a quenching experiment of 99% Al_2O_3 plate. Quantitative and stastical analysis shows that dimensions of cracks (length and direction) and numbers of cracks are similar to those in experiment for different temperatures. We further compared the cutting of an RC block using a LASER beam with experimental data. The cracking pattern in simulation results are in good agreement with those observed in experiment, which suggests the developed numerical model can be used study cracking induced by thermal shocks [2].

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Estimation of Occurrence and Displacement of Surface Fault Using High Performance Computing - Simulations of Surface Ruptures in Recent Earthquakes in Japan -

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Key Words: *Fault displacement, Surface rupture, High performance computing, Joint element, Finite element method*

As an aftermath of the great earthquakes that occurred in Taiwan and Turkey in 1999, there are concerns about structural damages that are caused by surface earthquake faults. Important facilities such as nuclear power plants are separated from the primary faults that extend directly from the epicenter. However, there are several sites where secondary faults are distributed under or near these important facilities. Estimating the occurence and displacement of the surface earthquake fault is an important issue for the safety assessment of such sites. Numerical simulation based on continuum mechanics has the potential to provide reliable estimates of fault occurence and displacement.

Numerical simulations of fault rupture processes pose the two significant difficulties. The first is that a huge amount of numerical computation is required to simulate the processes over a range of several hundred meters. The second is the loss of the stability of the initial and boundary value problem to which the numerical simulations are applied. The loss of stability here means that a small disturbance can cause a large change in the solution. In this study, we developed a parallel finite element method that implemented the following two functions: 1) symplectic time integration (explicit method) to properly conserve the energy of faults; and 2) rigorously formulated higher-order joint elements [1].

We applied the parallel finite element method to simulate two recent earthquakes which induced surface earthquake faults in Japan, 2014 Northern Nagano Earthquake (reverse faulting) and 2016 Kumamoto Earthquake (right lateral strike-slip faulting). The analysis model was constructed in a 5 km x 5 km x 1 km area including the primary and secondary faults. On the bottom of the analysis model, we applied the displacement bounday conditions which were calculated based on the elastic dislocation theory using the slip distribution on the main fault which was obtained from the inversion analysis. As a result, we succeeded to reproduce the occurence and displacements of surface faults observed in the two earthquakes. The rupture characteristics of the secondary faults in the simulations were different between the two earthquakes. The largest slip was computed at the ground surface or at the contact point with the main fault, respectively, for the simulation of 2014 Northen Nagano Earthquake simulation or 2016 Kumamoto Earthquake.

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Fast and Scalable Seismic Soil Liquefaction Simulation with Finite Element Method on GPUs

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Key Words: Large-scale Simulation, Finite Element Method, Soil Liquefaction

Three dimensional earthquake simulation has been expected to give us knowledge on the earthquake and the way to mitigate the damage from it. However, it entails huge computational cost, which makes it difficult to perform simulation for large domain with high resolution. To overcome the high computational cost, we have been developing fast and scalable earthquake simulation methods.

In this study, we developed a GPU-accelerated large-scale earthquake simulation method considering soil liquefaction [1] based on the CPU-based soil liquefaction simulation method [2]. We used the finite element method with second order tetrahedral elements solved with a conjugate gradient based solver that adopted the MPI-OpenACC hybrid parallelization. The developed method achieved a 10.7-fold speedup over the CPU-based method on a compute node of the GPU-based supercomputer, AI Bridging Cloud Infrastructure (ABCI). With the developed method, the computation time for the simulation with an 89,146,716-DOF soil-structure model over 30,000 time steps was 3 h 33 min using only 13 computing nodes on ABCI. When the CPU-based method was used, it took 14 h 37 min using 128 compute nodes on OFP to perform the same simulation. By using GPU, large-scale simulation can be performed with smaller computation environment with shorter computation time.

The reduction of computational cost of simulation by the developed method is expected to make it easier to carry out analyses that require multiple cases of simulation, such as Monte Carlo simulation for uncertainty quantification and data assimilation for parameter optimization. In addition, it is expected that more learning data for surrogate models can be generated and more accurate surrogate models will be constructed.

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High-resolution Seamless Simulations of Earthquake Disasters and Economy

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Key Words: agent-based economic modeling, post-disaster economy, high-performance computing

We developed an integrated system for estimating economic impacts of earthquake disasters by performing end-to-end simulations of disasters and economy at 1:1 scale. In order to realize 1:1 scale simulations, we developed a High-Performance Computing (HPC) extension for Agent Based Economic Models (ABEMs) [1] and seamlessly integrated it with physics-based earthquake disaster simulators [2]. It is demonstrated that the HPC extension has sufficient numerical efficiency and scalability to simulate a model with 330 million agents, which is equivalent to an 1:1 scale model of Euro-zone economy, within a few minutes using a few hundred CPU cores. The economic model is validated by reproducing major indices of Japanese economy for the period of 2015 to 2020. Due to the unavailability of the economic data of each individual entity, we generated data for 127 million economic agents by disaggregating the macroeconomic data available from several Japanese government agencies. Using Performance Assessment Calculation Tool (PACT), developed by the Federal Emergency Management Agency, USA, to estimate the direct losses and the repair time of each building, we seamlessly integrated the physics based disaster simulators with the developed ABEM. As a demonstrative application of the developed system, we estimate the economic impacts of a disaster in Hanshin industrial region caused by a potential Nankai-trough mega-thrust earthquake, and the disaster hit economy is compared with the normal state of the economy.

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Modeling Frameworks for Earthquake Deformation Problems

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Key Words: *Adjoint-based Optimization Methods, Inverse Theory, Dynamics of Crustal and Mantle Deformation, Earthquake Source Processes*

Advances in seismology and geodesy suggest that rock deformation surrounding earthquakes is affected by a range of transient processes deviating from Reid's simple seismic cycle model. In particular, observations from megathrusts including the disastrous Tohoku-oki 2011 M9 event have renewed interest in better constraining fault loading, and studies exploring if precursory signatures such as those often seen in the lab can be usefully exploited in nature for potential hazard assessment applications. Here, we address some of the challenges that remain for the integration of these multi-scale data into comprehensive numerical models. We ask how to best extract information to reduce uncertainties on any modeling-based estimates of megathrust state. For this, a multi-institutional team was recently funded by the US NSF to establish a Megathrust Modeling Framework (MTMOD), and we will highlight some of the participants' efforts in this presentation. One particular example of our efforts to move toward adjoint-based approaches for the static and time-dependent problems involved is a new, open-source finite-element framework to solve visco-elastic earthquake deformation problems. Based on two libraries for the forward and inverse problems, respectively, our new framework is flexible, transparent, and easily extensible to implement complex multi-physics coupled problems. FEniCS [1] offers a collection of software components for automated and efficient solution of PDEs, and hIPPYlib [2] state-of-the-art, scalable adjoint-based algorithms for deterministic and Bayesian inverse problems. Using this framework, we present a fault problem test case, representing the slip discontinuity with a mixed finite-element formulation. This approach solves for stress with higher order accuracy than typical approaches, and exposes the prescribed slip explicitly in the variational form without using split nodes or domain decomposition. Our formulation allows the optimality conditions, gradient and Hessian, to be expressed in continuous form, which leads to consistent discretizations of all field variables, including the slip. We show some applications of this new framework by inverting geodetic surface displacements to infer the coseismic slip distribution for earthquakes as well as the crustal and mantle material parameters. Moving beyond traditional Green's function, homogeneous medium approaches is important to understand the presence of fluids and poroelastic effects, for example, as likely reflected in time-dependent seismic velocity observations. More generally, this framework promises to allow exploring more general inverse questions, such as to the fault and rock constitutive behavior that best fits a range of observations. These efforts will be helpful in future optimal experimental design studies to provide answers and reduce the uncertainties for fundamental questions in earthquake science of societal relevance.

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Seismic Wave Simulation from Earthquake Fault to City with Large-Scale Finite-Element Analysis on Fugaku

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Key Words: *finite-element method, high-performance computing, fault-to-city earthquake simulation*

Finite-element analysis with low-order unstructured elements is suitable for earthquake simulation from fault to city for considering the complex 3D geometry and nonlinear material heterogeneity. However, such simulation entails huge computational cost as the target domain is large and the required time-resolution for assessing structural damage is high. Thus, we have been developing fast and scalable finite-element solvers suitable for large-scale supercomputer systems. In this talk, we will introduce our recent developments in implicit low-order unstructured finite-element solvers suitable for supercomputer Fugaku, which is the fastest supercomputer as of June 2021 Top 500 ranking. Here we developed methods to efficiently utilize SIMD units and many-cores of Fugaku's Arm A64FX CPU [1], and developed methods to use data acquired in past time steps to accelerate solving of the next time steps [2]. This solver is scalable to nearly full system of Fugaku (147456 compute nodes) with performance of 9.97% of FP64 peak, which corresponds to 59.2-fold speedup from the previous state-of-the-art solver running on the full K computer system, which is the previous flagship supercomputer in Japan. As the hardware performance ratio between K computer and Fugaku is 46.9-fold, we can see that effective speedup was obtained by suitable algorithm and implementation development. Using the developed solver, we show a fully-coupled fault-to-city earthquake simulation where wave propagation from fault to city, wave amplification at ground near surface, and structural response is computed using a monolithic mesh with 324 billion degrees-of-freedom with resolution varying from 0.125 to 64 m. Such simulation is expected to be useful for explicit evaluation of nonlinear coupling effects between earthquake subprocesses, which are difficult when computing each subprocess separately.

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Study on Seismic Response Analysis of Large-Scale Reinforced Concrete Structures Using High-Fidelity Models

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Key Words: *Large-Scale Reinforced Concrete Structure; High-Fidelity Model, Seismic Response Analysis*

For seismic response analysis of important facilities such as nuclear power plant buildings, it is effective to use a high-fidelity model with solid elements due to its higher reliability compared with a lumped mass model. When analysing the seismic response of large-scale reinforce concrete (RC) structures using high-fidelity models, high-performance computing (HPC) is indispensable because of the number of degrees of freedom (DOFs) especially in considering soil-structure interaction. This study shows the development of finite element method (FEM) for seismic response analysis of large-scale reinforced concrete structures utilizing HPC and a trial seismic response analysis of a nuclear power building model.

A key issue of development of HPC-FEM satisfying mensioned purpose is restriction of algorithms by its solver. We implemented a tensorial constitutive relation of concrete [1] [2] to the HPC-FEM program FrontISTR [3]. This constitutive relation employs an elasto-plastic and damage model, which expresses the damage to the material in terms of the softening of the stress-strain curve, results in the loss of positive-definiteness of elasto-plastic moduli at large deformation and prevents convergence of the conjugate gradient (CG) method, a solver of HCP-FEM. There are several non-linear analysis techniques or Newton method techniques for dealing with this problem; we adopted a method of calculating the stiffness matrix using elastic tensor of the material, which is a kind of modified Newton method, by comparing its speed and stability of computation with those of other methods. To check the performance, the developed software was validated by a simulated loading test of an RC structure. In this performance check, we also checked the performance of the CG method solver which changed by the non-linear analysis methods. It was shown that the non-linear analysis method using elastic tensor made the performance of the CG method solver higher and more stable.

Finally, we applied the developed method to the seismic response analysis of a nuclear power plant building with surrounding ground using high-fidelity model, which was a model of approximately 1.5 million DOFs. The results of the numerical analysis were discussed, focusing the numerical performance of HPC-FEM.

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Dynamic parameterization of a modified SEIRD model to analyze and forecast the outbreak evolution of COVID-19 in the United States

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Key Words: *COVID-19, mathematical epidemiology, modified SEIRD model, dynamic parameterization*

The COVID-19 pandemic has raised the interest and use of mathematical models to understand and predict infectious disease dynamics, which has contributed to the decision-making of public health authorities [1]. These models can be broadly classified into two groups. Statistical models may handle complex outbreak dynamics, but they heavily rely on data series and do not provide insight into the underlying mechanisms of COVID-19 contagion spread. Mechanistic models usually rely on a compartmental formulation that facilitates the representation of the mechanisms of disease transmission and contagion but they may require specific data on disease infection status and recovery that is not often available [2]. Also, they usually employ constant parameters for separate waves of the pandemic, limiting their ability to represent complex outbreak dynamics.

To exploit the advantages of both modeling paradigms, our work proposes a data-informed mechanistic approach that leverages universally available epidemiological data (i.e., cumulative infections and deaths) to provide a smooth time-resolved parameterization of the dynamics of COVID-19 spread. We employ a modified SEIRD model featuring symptomatic and asymptomatic contagion [3]. This model is initially fit to successive one-week intervals of cumulative infections and deaths over a given timeframe using constant parameters. Then, we apply a mean filter to obtain time courses of daily estimates of the model parameters, which we subsequently fit quadratic B-splines to render a smooth model parameterization for analysis and forecasting. We tested our methodology in five representative states of the US between March 2020 and August 2020 (NY, CA, IL, TX, and FL). At this endpoint, nationwide seroprevalence estimates were available, which we also use to estimate the proportion of recovered individuals during model calibration.

Our method results in a median [range] normalized root mean squared error (NRMSE) of 3.64% [1.68%, 7.96%] and 4.22% [1.38%, 6.20%] during calibration for cumulative infections and deaths, respectively. The corresponding 2-week forecasts result in an NRMSE of 3.48% [1.30%, 12.16%] and 4.70% [0.86%, 8.91%], while the 4-week forecasts render an NRMSE of 3.95% [0.91%, 43.90%] and 11.03% [0.96%, 35.26%], respectively. When the subsequent 2 weeks of time-series data are assimilated, the forecasting accuracy of our method increases, with the NRMSEs of the prior 4-week forecast decreasing to 1.67% [0.61%, 6.48%] and 1.52% [0.09%, 4.72%], respectively. The dynamic parameters obtained offer insights into key temporal mechanisms, such as the substantial reduction in contact rates following governmental lockdowns. Thus, we think that our methods can potentially be developed into a predictive technology enabling the forecast of time-resolved mechanisms of infectious disease spread to guide public health decision making, such as medical resource allocations and non-pharmaceutical interventions.

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3D-0D closed-loop model for the simulation of cardiac electromechanics including a detailed myofiber architecture

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Key Words: Cardiac electromechanics, Cardiac fiber architecture, Multiphysics modeling, Finite Elements, 3D-0D coupling.

Two crucial factors for accurate numerical simulations of cardiac electromechanics (EM), which are also essential to reproduce the synchronous activity of the heart, are: i) reconstructing the muscular fiber architecture that drives the electrophysiology signal and the myocardium contraction; ii) accounting for the interaction between the heart and the circulatory system, that determines pressures and volumes loads in the heart chambers. In this work, we present a 3D whole heart EM model coupled with a 0D closed-loop model of the whole cardiovascular system, that addresses the two former crucial factors. Our whole heart 3D-0D model includes a detailed myocardial fibers architecture, simulates the electrophysiology, the mechanical activation and the mechanics of ventricles and atria, and is strongly coupled with a 0D-closed loop model of the whole cardiovascular system. The main contributions in this work move along two strands: i) on the one hand, we developed a unified mathematical framework, based on Laplace-Dirichlet-Rule-Based-Methods (LDRBMs), to prescribe myocardial fibers orientation in computational full heart geometries [1]; ii) on the other hand, we provide a biophysically detailed 3D EM model coupled with a 0D closed-loop lumped parameters model for the haemodynamics of the whole circulatory system [2]. Specifically, we describe the whole heart LDRBM, which is able to quantitatively reproduce almost all the features of the different four-chambers. We also discuss in detail the coupling approach that stand behind the 3D-EM and the 0D-fluid models. Finally, we present physiological EM simulations, on a realistic whole heart geometry, using the 3D-0D model and we show that our results match the experimental data available in literature.

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A Parallel Algorithm for the Simulation a Patient-specific Heart with Four Chambers

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We consider the numerical modeling of the elastodynamic behavior of the whole human heart whose geometry is reconstructed from MRI images. We propose a parallel domain decomposition method for the numerical simulation of a patient-specific heart with four chamber and fibers. Because of the complex hyperelastic model, the complicated geometry, the fiber directions, and the active stress distribution, the solution of such a problem is very difficult to obtain. Our algorithm is constructed within the framework of the implicit Newton-Krylov-Schwarz method modified for this particular problem. Numerical experiments show that the algorithm is able to simulate the cardiac elastodynamic involving hundreds of millions of degrees of freedom on a supercomputer with more than 10,000 processor cores.

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Boundary Element Method for the Cell-by-Cell Model in Cardiac Electrophysiology

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Key Words: boundary element method, bidomain model, electrophysiology, time integration

In cardiac electrophysiology, electric potentials generated by muscle cells impact the correct heart operation. Muscle contraction, for instance, depends on the transmission of electric signals from cell to cell, which in turn are affected by structural muscle disease, ageing and cardiomyopathies. Therefore, heart modelling at the cellular level is crucial for the accurate simulation of abnormal hearts.

At microscopic scale, the cardiac tissue is composed by tightly coupled myocytes, embedded into an extracellular matrix and surrounded by other cells. The bidomain model is a system of partial differential equations describing the spatio-temporal evolution of the electric potential within each cell and in the extracellular space. In particular, the model accounts for the cellular membrane dynamics and cell-to-cell coupling at fine scale. From a numerical perspective, the bidomain model at microscropic scale, henceforth called "μ-bidomain model", poses a number of difficulties: the cellular subdomains are separated by a sharp interface, that is the cellular membrane; the temporal dynamics, dictated by the membrane ionic model, is confined on such interfaces; and the membrane dynamics is typically nonlinear, multiscale and severely stiff in time. Therefore, the electric potential is globally discontinuous and the PDE is degenerate in time, due to the elliptic constraints.

In this work, clear away the uninteresting intra- and extra-cellular Laplace equation recasting the μ-bidomain model into a boundary integral formulation and employ the boundary element method for the space discretization. This yields a time dependent system living on the cellular membranes only, where the interesting dynamics occur. We analyse the local well-posedness of the reaction-diffusion system. Furthermore, we compare the efficiency of various families of time discretization schemes: implicit-explicit schemes, Rush-Larsen schemes, explicit stabilized (Chebyshev) Runge–Kutta methods, multirate methods.

Finally, we present some numerical experiments to compare the boundary integral formulation to a more standard finite element approach. We also discuss the feasibility of the approach towards the application to large scale models.

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Efficient and robust parallel solvers for cardiac reaction-diffusion models

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Key Words: Cardiac Bidomain model, scalable parallel preconditioners, high-performance computing, nonlinear solvers.

The Bidomain model provides a mathematical description of the electrical activity in the heart. Its numerical solution still represents a challenging task for the scientific community, due to the coupling of macroscopic and microscopic phenomena (the propagation of the electric signal in the cardiac tissue and the ionic currents dynamics at a cellular level, respectively). Indeed, balancing accuracy in the solution of the system arising from discretization of such models while being computationally competitive (in terms of scalability and efficiency) is an actual issue which can be overcome with the development of specific techniques.

In this work, we present a numerical comparison of several parallel solvers for the numerical simulation of the Bidomain equations. We focus on a finite element discretization in space and different schemes for the time discretization, leading to the solution of large algebraic systems. Iterative methods are considered for their solution, where fast convergence is ensured by preconditioning with suitable algorithms. Whenever nonlinear algebraic systems arise, nonlinear solvers are employed, such as inexact Newton, quasi-Newton and nonlinear Generalized Minimal Residual methods.

We investigate strong scalability and robustness of the resulting solvers through extensive parallel numerical tests. These preliminary results provide a basis for further studies of parallel solvers for cardiac electrophysiology models that combine parallel efficiency while yielding accuracy in the solution and exploiting modern computational architectures.

This is a joint work with Nicolás A. Barnafi (Univ. of Pavia), Simone Scacchi (Univ. of Milan) and Luca F. Pavarino (Univ. of Pavia).

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Efficient and Scalable Solvers for Cardiac Mechanics

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Key Words: Cardiac mechanics, Scalable preconditioners, Domain Decomposition, Nonlinear solvers

The development of realistic cardiac models is an active area of research, with the numerical approximation of these models being a great computational challenge. The main bottleneck is the repeated solution of large-scale and ill conditioned linear systems of algebraic equations arising from Newton's method, which require scalable preconditioners to obtain efficient iterative solvers. The most well-established iterative method for this aim is the GMRES algorithm, preconditioned by the Algebraic Multigrid (AMG) method. The AMG preconditioner is widely popular as it provides a black-box solution for preconditioning that works most of the time, but there are certain aspects that do not perform optimally, such as higher order elements, and it requires setting a plethora of parameters. Balancing Domain Decomposition by Constraints (BDDC) methods provide an alternative to AMG methods, which in classic linear problems have been shown to provide quasi-optimal conditioning, verified up to hundreds of thousands of parallel processors.

In this talk we will explore Newton, inexact-Newton and quasi-Newton methods for cardiac mechanics in detail. We start this by providing a detailed study of the performance of the BDDC preconditioner, where the advantage of considering this preconditioner instead of AMG will be shown through numerous tests. After this, we study the performance of alternative nonlinear solvers for the root-finding problem of solving the Euler-Lagrange equations associated to the mechanics. We focus on superlinearly convergent solvers, namely quasi-Newton BFGS and inexact-Newton, and show that (i) between them there is no clear winner in terms of performance, so that the method of choice is problem dependent and that (ii) in all cases, little effort is required to obtain a method that is not only faster than Newton, but also robust and scalable.

This is a joint work with Simone Scacchi (University of Milan) and Luca Pavarino (University of Pavia).

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Higher-order time integration with algebraic adaptivity in a cell by cell discretization of cardiac excitation

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Key Words: cell-by-celll discretization, high-order time integration, spectral deferred correction, algebraic adaptivity

Cardiac arrhythmia causes about 15% of all mortality, primarily due to disorganization of cardiac tissue at the cellular scale, impacting the propagation of myocardium excitation. In order to understand disease mechanisms, diagnose illness, and design effective drugs for treatments, numerical modeling at the cellular level is necessary.

The most exact electrophysiological models, such as bidomain and monodomain models, represent the action potential on the tissue level, which can not describe details of propagation at the cellular level. We reformulate the electrophysiological model on the cellular level, with separate extracellular intracellular domains separated by cell membranes including ion channels and gap junctions.

We discuss the cell-by-cell model of cardiac excitation from [1] and its discretization with arbitrary order finite elements in space and arbitrary order time stepping with spectral deferred correction methods (SDC) [2]. A shrinking effective support of SDC corrections allows for a reduction of the spatial domains on which Euler subproblems need to be solved. The adaptive subset selection on the algebraic level leads to a natural multirate integration scheme, which results in reduced computational effort. The effectivity of this approach and the resulting efficiency in terms of computing time and energy consumption is illustrated at some numerical examples.

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Simple Tools for Cardiac Simulation GPU-Parallel Nonlinear Multiphysics

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Key Words: Multiphysics Problems, Cardiac Simulation, Electrophysiology, Mechanics, Fluid Dynamics, Fluid-Structure Interaction, GPU, Parallel Computing

Given the social and economic cost of cardiovascular disease, the value of in-silico cardiac simulation is self-evident, with applications in both clinical and research fields. There are established models for the various aspects of cardiac function, each operating at different scales in space and time. The key challenge of whole heart simulation is to combine of these models in a way that is both physically accurate and computationally feasible, with respect to both time and processing resources.

The aim of this work is to provide a simple computational framework which unifies these mathematical models into a single discretisation and processing environment without software dependencies, such that multiple cardiac simulations can be configured and generated by a clinician or researcher within minutes or hours on a single desktop processor.

The PDEs that represent the physical processes that propagate the wave of depolarisation through the myocardium (Mitchell-Schaffer and Monodomain Equations), leading to muscle contraction (Hyperelastic Finite Strain) and pressure changes that generate blood flow (Incompressible Navier Stokes) are integrated in space and time via techniques from Finite Volume and Finite Difference methods. Fluid-structure interaction is modelled via the Arbitrary Lagrangian-Eulerian approach.

The simulation environment consists of a set of scalar, vector and tensor fields discretized over a three-dimensional regular structured grid. Differential operators are assembled in matrix-free form into a set of computational kernels, which are processed in parallel on a Graphics Processing Unit. The solver handles each part of the problem in turn within a single computational loop, passing three-dimensional buffers containing physical quantities through a stream of parallel computation. The resulting software tools are simple enough to re-used by students, researchers and clinicians for a wide variety of valuable investigation.

The presentation will demonstrate the convergence of the discrete operators at each step of the computation and reproduce benchmarks for electrophysiology, solid and fluid dynamics, as well as show examples of more complex cardiac function.

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Stabilizing numerical oscillations in cardiac active mechanics: an oscillations-free and accurate fully partitioned scheme

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Key Words: Coupled problems, Cardiac modeling, Multiscale modeling, Active stress, Numerical stability

In this work we address an unresolved problem in the numerical modeling of cardiac electromechanics, that is the onset of numerical oscillations due to the dependence of force generation models on the fibers shortening velocity. A way to avoid numerical oscillations is to use monolithic schemes for the solution of the coupled problem of active-passive mechanics. However, staggered strategies, which foresee the sequential solution of the models of force generation and of tissue mechanics, are preferable, due to their reduced computational cost and low implementation effort. In light of this motivation, in this work we propose a new numerical scheme, that is numerically stable and accurate, yet within a fully partitioned (i.e. segregated) framework [1]. To derive our stabilized scheme, we move from energetic considerations on the coupling, at the microscale, between active and passive mechanics models. We show that instabilities are linked to the mismatch between macroscopic and microscopic strains, inconsistently expressed in Lagrangian and Eulerian coordinates, respectively. Hence, we formulate a novel scheme, in which all the variables are framed in a coherent fully Lagrangian reference system. By considering a model problem of active mechanics we prove that the proposed scheme is unconditionally absolutely stable (i.e. it is stable for any time step size), yet within a fully staggered framework. We apply the proposed method to several force generation models available in the literature, namely the Niederer-Hunter-Smith model, the model of Land and coworkers and the mean-field model that we proposed in [2]. We show, by means of several numerical tests, that the proposed stabilization term successfully removes the nonphysical numerical oscillations characterizing the non-stabilized segregated scheme solution. This is verified in several test cases, including a three-dimensional multiscale electromechanical simulation of the left ventricle. We show that the new scheme preserves the first order convergence with respect to Δt of the non-stabilized staggered scheme. The numerical error is only slightly larger than the error obtained with the monolithic scheme and it tends to zero with the same rate.

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Numerical stabilization for the constraint formulation of many-body-many-contact Coulomb friction

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Key Words: Many-body Coulomb friction, Constraint mechanics, Differential-algebraic system, Discrete element method, Numerical stabilization

We have formally solved the Coulomb friction problem for many-particle multiple-contact systems in two [1] and three [2] dimensions. The discrimination between static or dynamic friction is based on the relative accelerations, projected onto the contact. So the problem is effectively one-dimensional and the formalism by Hairer et al.[3] for differential-algebraic system with unilateral constraints can be applied: The relative accelerations at each contact can be computed independently from the convex hull with both friction directions and be converted into forces via the tangential reduced mass.

The issue we treat here is the additional noise due to discretization errors for simulations with finite timestep. They lead to numerical drift away from the constraint, becoming effectively a vibrating force which dislocates particles from their equilibrium positions. In numerical analysis, the standard approach to prevent drift in constraint systems is via "stabilization by projection" (of the coordinates or velocities) into the constraint manifold [4]. However, for many-body multiple-contacts systems like discrete element methods, this is not feasible, as there can be simultaneously more than one constraint manifold. We will explain alternative stabilization approaches as well as the effects of different stiff integrators.

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Texture Shape Optimization for Minimization of Friction Coefficient (Comparison of Shape Optimization Results for Circular and Herringbone Textures)

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Key Words: *Shape Optimization, Adjoint Variable Method, Finite Element Method, Friction Coefficient, Circular Texture, Herringbone Texture.*

In this study, we present numerical results of the texture shape optimization analysis for minimization of frictional force (cf. [1], [2].). The Reynolds equation is introduced as the governing equation, and is discretized in space by the finite element method. The performance function is defined by the frictional force. Also, the purpose of this study is to find the distribution of oil film thickness in the textured area, i.e., the design variables, so as to minimize the performance function. Here, it is necessary to consider the governing equations as constraints on the performance function. Therefore, the adjoint variable method is introduced to derive the Lagrange function. In order to obtain the stationary condition for the Lagrange function, the first variation of the Lagrange function is calculated. Finally, the gradient of the Lagrange function with respect to the design variable is obtained, and the iterative computation is performed to obtain the optimal solution for the design variable. In this study, we perform shape optimization analysis for the circular texture and the herringbone texture models, and present some numerical results (See Fig.1.).

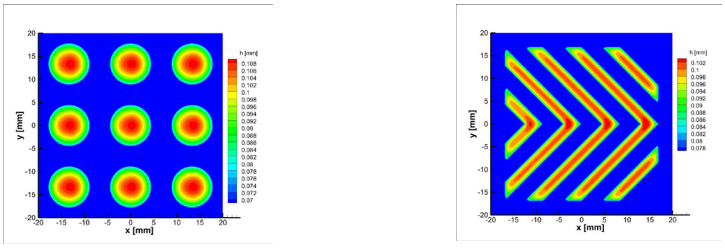

Fig.1 Comparison of optimal oil film thickness at texture parts in case of circular and herringbone textures

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An efficient single-loop method for structural design under the random uncertainties with interval distribution parameters

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Key Words: *Reliability-based design optimization (RBDO); Imprecise probabilities; Probability-interval hybrid uncertainty; Single-loop method.*

The Reliability-Based Design Optimization (RBDO) provides an effective way to obtain the optimum design in the presence of random uncertainties which follow the precise probability distribution function in the structural optimization design. However, in many practical engineering problems, the probability distribution which describes the stochastic nature of the uncertainties cannot be precisely obtained due to limited information. To quantify this kind of imprecise uncertainties, a probability-interval hybrid model emerged, where all uncertain variables are treated as random variables while some distribution parameters can only be given variation intervals. For such kind of uncertainties, this paper establishes a hybrid RBDO model and proposes a single-loop solution algorithm. The outer loop of the hybrid RBDO is performed to find the optimum design and the inner loop of that is performed to assess the reliability. However, the interval parameters lead to an interval of reliability for each constraint function, thus giving rise to a double-loop problem for the inner loop. Therefore, solving the hybrid RBDO would encounter the unaffordable computational effort and the hinder of convergency due to the nested strategy. In this paper, the Karush-Kuhn-Tucker (KKT) optimality conditions of the inner loops are imposed as equivalent deterministic equality constraints. The original triple-loop optimization is thus converted into an equivalent single-loop problem, which alleviates the computational demand significantly. The efficiency and accuracy of the proposed single-loop method (SLM) is verified through several practical engineering problems.

Identification of Key Parameters of Nonlinear Friction of Robot Joints based on Neural Network

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Key Words: *Robot, Parameter identification, Nonlinear friction model, Neural network, Friction compensation*

Accurate identification of nonlinear friction parameters in robot joints is the linchpin to the trajectory and positioning accuracy as well as the kinematic stability of the arm-tip of robot during operations. However, it is not straightforward to derive these parameters exactly due to the complexity of the robot system. To this end, this study develops an inverse method through a neural network for determining the key parameters of nonlinear frictional torque model for robots. Specifically, the friction parameters of the robot joint are measured by a constant speed tracking experiment. The robot dynamics model containing nonlinear friction was established to calculate joint torques. The excitation trajectory is designed and the sensitivity of friction parameters to joint torques is analyzed to determine the key friction parameters. Then the optimal Latin hypercube method is used to sample in the friction parameter space. A neural network is subsequently established with 6 inputs produced with the robot dynamics model and 3 outputs generated by sampling. The friction model is established by using the friction parameters identified by the neural network to compensate the friction torque of the robot in the simulation experiment. The predicated friction parameter using the currently proposed identification method are accurate with the maximum test errors less than 0.4%. It can effectively improve the influence of the abrupt change of the friction torque on the trajectory of the robot when the robot moves in low speed and the trajectory accuracy of the robot is greatly improved.

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Multi-objective Optimization of 1-DOF Transformable Wheel Mechanisms for High Adaptability

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Key Words: *Kinematics, Transformable Wheel, Performance Index, Initial Contact Angle, NSGA-II Algorithm*

A transformable wheel is a critical mechanical component in a mobile robot climbing up or down step obstacles of various heights. In the case of a tri-segmented transformable wheel to be considered here, it changes the effective radius and tilting angle of the three wheel segments for stable locomotion possibly with high energy efficiency. This study presents a multi-objective kinematic profile optimization of a one-degree-of-freedom (1-DOF) transformable wheel mechanism for highly adaptive locomotion. Compared with available 2-DOF wheel mechanisms [1, 2], the 1-DOF wheel mechanism has critical advantages in cost, weight, and actuator control. If 1-DOF wheels are designed for a step obstacle of a specific geometry, however, they cannot be directly used for other step obstacles of different widths and heights because they do not have sufficient DOFs. To address this critical issue, we propose to employ the initial angle of contact between the wheel and a step as a new additional variable. We show that this idea enables us to establish a one-to-one mapping between configurations of the wheel shapes and the target obstacles of any geometry. Here, the initial contact angle is defined as the pre-rotated angle at the moment of the climbing. By using one variable to transform the wheel and an additional variable of the initial contact angle, the transformable wheel can overcome various obstacles. However, the 1-DOF mechanism cannot represent all deformation shape because the profile of radius and angle are co-related unless the wheel is so transformed to follow an elaborate locomotion planning. This planning problem can be set up as an optimization problem where the wheel acceleration is minimized, and its instability is maximized for adaptive step-climbing. We employ the nondominated sorting genetic algorithm-II (NSGA-II) [3] to identify a Pareto-optimal front and examine the trade-off relation between performance indices. In order to analyze and design the movement of the transformable wheel, we use a simplified forward kinematics model. Finally, we present the 1-DOF optimal profiles utilizing a successfully configured Pareto-optimal front. The experiment results using an actual robot platform will be demonstrated.

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Comparing study on acoustic problems in uniform subsonic flow based on the fast multipole boundary element method

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Key Words: *Acoustics, Uniform Subsonic Flow, Fast Multipole Boundary Element Method*

The boundary element method (BEM) is an effective numerical tool for the calculation of acoustic radiation problem in infinite domain. Due to the addition of convection terms, the convective wave equation for uniform mean flow and its Green's function form are more complex than the traditional form[1]. Two technical routes have taken the mainstream for the use of the boundary element method in uniform mean flow fields. One is to directly substitute the convective Green function into the boundary integration equation in the stationary coordinate system[2], and the other introduces the approximate Lorentz transformation, which converts the wave equation and the Green function into the traditional concise form for quiescent medium and then substitutes the boundary integral equation[3].

The fast multipole acceleration for the above two techniques for acoustic problems in uniform subsonic flow are presented. The first and second use the Green's function in the rest frame and the Green's function in acoustic analogue Lorentz space as the FMM kernel, respectively. The radiation of a pulsating sphere in uniform subsonic flow with analytical solution is considered as a benchmark to test the performance of the two methods. CPU time, accuracy and convergence are included as the primary performance measures in the study. Two methods are investigated for the benchmark problem with different frequencies (from 5Hz to 200Hz), Mach number (from 0.01 to 0.9) and model scale (from 500 elements to 600000 elements). The comparison of the results of both methods shows that almost the same accuracy is achieved on the small scale, low-frequency problems. However, higher computational efficiency is witnessed due to the concise form of the kernel in the method using the Green's function in acoustic analogy Lorentz space. A possible improvement of the algorithm is also discussed based on the characteristics of sound propagation in the uniform subsonic flow.

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Damping Uncertainty and Sound Transmission Loss of Laminated Composite Plates with Embedded Damping Layers

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Laminated composite structures have been widely applied in the engineering field due to their excellent performance such as light-weight and designability compared to traditional metal ones. Embedding the viscoelastic damping layers into the laminated composite to construct co-cured composite damping structures provides an effective way to improve the sound insulation capability. However, co-cured composite damping structures are inevitably subject to various uncertainties, which may come from manufacturing errors, environmental variability and simplified damping model. In this study, the sources of damping uncertainty of composite laminated structures with embedded damping layers are briefly discussed, and experimental tests by employing a number of cantilever beams with embedded a damping layer are carried out to demonstrate the uncertain damping properties of the damped composite structures. Furthermore, a semi-analytical model is proposed to investigate the sound transmission loss (STL) of a composite laminated plate with embedded viscoelastic damping layer subject to uncertain parameters. The results show the important effects of uncertain damping loss factor of a composite laminated plate on its STL valleys and peaks.

Key Words: *Composite laminated structure, Sound transmission loss, Damping layers, Uncertainty analysis*

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