Introduction by Chairman

The 6th African Conference on Computational Mechanics (AfriComp6) took place in Cape Town, South Africa, 26 – 28 February 2024. The first AfriComp has been held in Sun City (South Africa) and subsequently in Cape Town (South Africa), Livingstone (Zambia), Marrakech (Morocco) and returned to Cape Town in 2022. AfriComp6 has been organized by the University of Cape Town under the auspices of the South African Association for Theoretical and Applied Mechanics (SAAM), the European Community on Computational Methods in Applied Sciences (ECCOMAS) and the International Association for Computational Mechanics (IACM).

AfriComp's main objective is to provide a forum for researchers and students in computational mechanics on the African continent to interact with members of the computational mechanics community from around the world. In this way, the conference series is seen as a key initiative aimed at promoting computational mechanics in Africa.

AfriComp6 received excellent support by researchers and practitioners all across South Africa, with authors being drawn from numerous research and industrial organisations. The technical programme comprised topics from the wide range of applied mechanics and mathematics including structural mechanics; fluid mechanics; biomechanics; damage and fracture mechanics; multi-scale mechanics; multi-physics; advanced numerical methods; optimisation and design; big data and machine learning; manufacturing and process engineering. This Book of Abstracts contains the scientific contributions presented at the conference. Only original contributions were considered for inclusion.

Special acknowledgments are due to our supporters and partners in the industry:

- FEAS
- QFINSOFT
- FLOWNEX
- Journal of Mathematical and Computational Applications

Finally, the editor wishes to thank the authors for their efforts towards producing and delivering papers of high standard creating a base for discussion and providing suggestions for future development and research.

Sebastian Skatulla
Editor

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Programme

Overview

SUNDAY 25/02/2024. 17:00 – 18:30: Registration and Welcome Function, GSB (V&A Waterfront)		
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Session	**Venue A**	**Venue B**
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Tea Break (10:00 – 10:30)		
2 (10:30 - 12:30)	**Flow Problems**	**Structural Mechanics, Stability and Dynamics**
Lunch (12:30 -13:30)		
3 (13:30 – 15:30)	**Multi-scale and Multi-physics Problems**	**Damage, Fracture and Failure**
Tea break (15:30 – 16:00)		
4 (16:00 – 17:30)	**Transport Phenomena in Micro/nanofluids**	**Manufacturing and Process Engineering**
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7 (13:30 - 15:30)	**Data Science and Machine Learning (1)**	**Computation Modelling Biological Soft Tissues (1)**
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11 (13:30 - 15:00)	**Numerical Simulation Methods (1)**	**Coupled and Contact Problems**
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Monday, 26 February 2024

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Conference Opening: **Sebastian Skatulla, Chairman AFRICOMP, University of Cape Town**

Welcome Address: **Daya Reddy, Interim Vice-Chancellor, University of Cape Town**

KEYNOTE LECTURE

Ntobeko Ntusi, **University of Cape Town,** *Cardiovascular Strain Imaging - Impact on Clinical Decision Making*

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A new implicit fan model for robust air-side heat exchanger simulation *Adam Venter; Michael Owen; Jacques Muiyser*	**A hierarchical Snap-through model for Mimosa Pudica leaf folding kinematic** *Fabio Bazzucchi*
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Comparative Analysis of Lubrication Approximation and SPH-DEM Coupled Simulations for Rotating Drum Flows *Taswald L. Moodley; Indresan Govender*	**Modeling and Experimental Study of Eccentricity in Two-Stage Spur Gear Systems** *Yakeu Happi Kemajou Herbert; Bernard Xavier Tchomeni Kouejou; Alfayo Anyika Alugongo*
Simulating blood flow through pathological aortic valves using reduced order modelling, 3D CFD simulation and experimental approaches *Lindi Grobler; Ryno Laubscher; Johan van der Merwe; Philip G. Herbst; Daniel Harrison*	**Progressive Analysis of a Nonlinear Electromechanical System Sensitive to Initial Conditions by the Poincare Method** *Bernard Xavier Tchomeni Kouejou*
Presentation by QFINSOFT	**Investigating Robustness to Instability Against Imperfections of a Gridshell Roof in Dakar** *Jonathan Melchiorre; Amedeo Manuello Bertetto; Giuseppe Carlo Marano; Fabio Bazzucchi*
	Dynamic Responses of Dielectric Elastomer Structures *Weiqiu Chen*

Lunch (12:30 -13:30)

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Tuesday, 27 February 2024

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Chris Rycroft, University of Wisconsin-Madison, USA, *The reference map technique for simulating complex materials and multi-body interactions*

Tea Break (10:00 – 10:30)

Session 6 (10:30 – 12:30)

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Conference dinner 19:00, Quay 4 Restaurant, V&A Waterfront	

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Investigating the Effectiveness of three mixing Techniques by Quantifying Dispersion and Homogeneity of CNTs/Ti6Al4V(ELI) powder mixtures using Image Analysis
Mpho Mashabela; Maina maringa; Thywill Dzogbewu

Development and preliminary numerical investigations of a dislocation density-based finite-strain rate-dependent elastoplasticity constitutive model
Emma Garschagen; Benjamin Alheit; Ernesto Ismail; Sarah George

Exascale Materials Calculations From First-Principles
Jerry Bernholc

Central Pattern Generator for Pneumatic Soft Robots
Martin Venter; Johannes Vegter</td><td>Adhesion and Friction: a Survey and a Unified Formulation
Michel Raous

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Anastasia P. Bogdanova; Anna A. Kamenskikh; Yuriy O. Nosov

Numerical identification of constitutive relations of viscoelastic and viscoplastic of lubricants behavior
Anastasia P. Bogdanova; Anna A. Kamenskikh; Yuriy O. Nosov

A Weakly-Compressible Two-Phase Formulation for Hydrogen Containment Modelling
Yusufali Oomar; Arnaud Malan; Francesco Gambioli

Magnetically induced blunt objects: Magnetohydrodynamic approach.
Thokozani Kunene</td></tr>
<tr><td colspan="2">Lunch (12:30 -13:30)</td></tr>
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Abstracts

1. Biological Systems

Understanding the Role of Flow on Clot Formation in COVID-19

Qudus Jimoh-Taiwo[1]; Weihua Ho[2]; Malebogo Ngoepe[1]
[1]University of Cape Town
[2]University of Witwatersrand

Coronavirus disease 2019 (COVID-19) is usually characterized by unprecedented clinical pathologies. Major features of the virus included increased clotting and inflammation, particularly in patients who develop severe illnesses. Altered clotting and inflammation remain important features in long-term COVID cases. Although inflammation has an influence on multiple processes, a notable effect of COVID-19 infection is aggressive intravascular thrombosis, on both the macro- and microscale. Most COVID-19 thrombosis studies to date do not include systemic and comprehensive investigation protocols; hence, the true prevalence of thrombosis associated with COVID-19 is unknown. Overall, the increase in thrombosis rate during COVID-19 conceivably lies in the confluence of three processes: firstly, endothelial inflammation; secondly, altered blood flow and blood composition; and thirdly, break-off of clots in the macrovascular system and subsequent congestion in the microvascular system. In previous work, the effect of isolated COVID spike protein on clot formation and blood flow was studied experimentally. COVID-19 thrombosis has been observed in both the macro- and microvasculature, with different effects. This work attempts to understand this difference by developing a computational model of thrombosis during COVID and then applying the model to both micro- and macroscale geometry. The model is validated by microfluidics analysis performed by Grobbelaar et al. A microfluidic vessel is used to simulate and investigate clot formation under flow conditions. The model is developed on ANSYS Fluent. Navier-Stokes equations account for the blood flow in the vessel. A multispecies approach is applied, where each of the biochemicals involved in clotting is simulated as an individual species. The species react with one another at the reaction rates defined by the Michaelis-Menten equation, leading to fibrin formation. A gradual increase in fibrin concentration allows for the formation of a fibrin mesh, which later becomes a clot. The fibrin mesh is modeled by varying the porosity of cells where the mesh is present. The formed in-silico clot is compared to the in-vivo clot formed during the microfluidics analysis.

Numerical and Experimental Assessment of Multi-Morphology Bone Tissue Engineering Scaffolds

Mikhail Tashkinov[1]; Natalia Elenskaya[1]; Yulia Pirogova[1]; Aleksandr Shalimov[1]; Ilia Vindokurov[1]; Vadim V. Silberschmidt[2]

[1]Perm National Research Polytechnic University

[2]Loughborough University

One of the current trends in biomedicine is the transition to personalized solutions as most suited to specific needs of a patient. A new paradigm has recently emerged for the design of biomedical devices thanks to the latest developments in the area of additive manufacturing (AM) technologies. The shape freedom offered by AM makes it possible to develop biocompatible structures that can be used for replication, regeneration, and maintenance of the functionality of human tissues as well as for creating prostheses, implants, scaffolds, and other biomedical devices. AM allows the production of components and structures not only with a specific shape and pre-defined architecture but also with unique combinations of topological (curvature), mechanical, transport (permeability, thermal conduction) and biological properties. In this regard, there is a need to develop approaches for the rational design of biomedical devices, based on the fundamental principles of physics and mechanics, experimental and theoretical studies, as well as multiscale computational models. This work presents benefits of AM for design of bone-tissue engineering scaffolds with optimal physical, mechanical, and biological properties. The results of comparative analysis of mechanical behaviour of the polymer lattice scaffolds designed according to different approaches and manufactured with the fused filament fabrication technology are presented. The scaffolds with a controlled continuous gradient structure were suggested for regeneration of bone tissue with changing porosities [1]. The combination of cells with different morphologies and porosity levels makes it possible to mimic the transition between various – trabecular and cortical – types of bone tissue, thus allowing the replacement of the damaged area at the tissue interface. Additionally, a novel approach based on growth of multiple cracks is offered for simulation of fracture in bone tissue and artificial scaffolds. The numerical results for mechanical models of the designed structures are compared with the original experimental data.

References

[1] N. Elenskaya, M. Tashkinov, I. Vindokurov, Y. Pirogova, V.V. Silberschmidt, Understanding of trabecular-cortical transition zone: Numerical and experimental assessment of multi-morphology scaffolds, J. Mech. Behav. Biomed. Mater. 147 (2023) 106146. https://doi.org/10.1016/j.jmbbm.2023.106146

A design process for a wearable hand-assistive soft robotic device allowing flexion and extension for different hand sizes

Sung bok Chung[1]; Martin Philip Venter[1]
[1]Stellenbosch University

A review conducted in 2021 on assistive hand exoskeletons for rehabilitation identifies that soft robotic gloves presented little to no consideration for the influence of joint forces and contact interaction between the human finger and soft robotic actuators, depending primarily on control strategies used to fit one hand while performing a specific motion. Such limitations provide restrictions when performing desirable rehabilitation exercises, such as tendon gliding which require varying kinematic configurations of the fingers. Moreover, the necessity for actuator designs to be tailored to individual patients, considering a range of hand dimensions, still needs to be considered to make actuator design more relevant for patient-specific analysis. This work aims to contribute to the field by creating a design environment focused on assessing the bending behaviour of a finger-actuator interaction using Finite Element Analysis (FEA) and musculoskeletal simulation means. The objective of this study is to establish predictive models capable of determining joint rotational stiffness coefficients, allowable reaction moments at joints, and pressure control adjustments for a soft actuator design. The final aim is to be able to determine how an actuator should be controlled to achieve a set of tendon gliding exercises for different hand dimensions. This study explores the influence of design modifications on a soft actuator design, the pneumatic network actuator (PneuNet). These modifications involve changes to the design and select parameters of the PneuNet, and their effects are evaluated using a fixed finger model making use of mean finger measurements found in the literature. A comparison is made between results achieved through a gradient-based optimization approach for performing tendon-gliding exercises and those obtained through intuitive and empirical methods. Consequently, this research creates a means to initially determine actuator design feasibility in achieving tendon gliding exercises for a single finger, thereafter, making considerations for actuator control adjustments needed for varied finger anthropometry. The theory of response surface methodology is used to study the effect of alterations made to finger measurements where data points are collected using a central composite design sampling scheme to fit and evaluate first and second-order response surface models. The bi-directional PneuNet was determined to be capable of achieving the kinematic orientation required for two different tendon-gliding exercises, performing full extension for fingers and a straight fist. Different FEA modelling schemes are investigated providing a comparative study on incorporating 2D, 3D reduced and full finger models and its effect on computational cost and deviations observed in accuracy for reduced modelling schemes. The actual observed bending behaviour of the standalone soft actuator, capable of achieving a specific set of tendon gliding exercises, will be presented, comparing results to its simulated bending behaviour to validate results.

The improved mechanical characterization of soft tissues including mounting preloading

Igor Karšaj[1]; Toni Škugor[1]; Lana Virag[1]
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Finite element (FE) modelling has become one of the main tools necessary for the better understanding of various cardiovascular systems from a mechanical point of view. The accuracy of FE simulations significantly depends on accuracy of material parameters which are obtained via mechanical characterization process. The latter consists of experimental testing and material parameters estimation using the optimization algorithm. When it comes to soft tissues, the go to type of experiment is planar biaxial tensile test, due to its resemblance of in vivo conditions and anisotropy of the tissue. In general, the sizes of soft tissue specimens available for experimental testing are usually small and highly compliant. During the mounting process of specimens on the testing machine, they are often slightly preloaded to avoid sagging and to ensure perpendicular orientation with respect to loading axes. Application of this initial load results in stress state that differs from the reference configuration and leads to the pre-stretching of the specimen which cannot be measured. This error further extends to the material parameters estimation. Described behavior is often neglected by disregarding pre-stretches or by manually annulling initial loading. Obviously, neither of the cases corresponds to the real stress and stretch state. In order to include pre-stretches in mechanical characterization we have developed a new computational procedure. Since experimental Cauchy stress is determined inaccurately, additional configuration that represents pre-stretched specimen in a state prior to the experiment has to be introduced. This is achieved with a supplementary nested loop that will iteratively calculate and correct pre-stretches to satisfy the equilibrium between initial experimental and model stresses. The verification of the procedure was done on the series of FE simulated virtual planar biaxial experiments where the exact material parameters could be set and compared to the obtained ones. Gasser-Ogden-Holzapfel (GOH) strain energy density function was used to model the tissue with material parameters being taken from the literature [1]. Furthermore, we have applied our procedure on the data gathered from biaxial experiments on aortic tissue and compared it with the results obtained through standard optimization procedure. The analysis has shown significant difference between obtained material parameters, especially in cases where GOH structural parameters such as fiber family angle and in-plane dispersion are considered as fitting parameters. The rate of error increases with the amount of applied pre-stretches and also decreases with increase of maximum achieved experimental stretches. Finally, annulling initial force proved to be better approach if only standard optimization is to be applied.

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Viscoelastic Modelling of Left Ventricular and Septum Myocardia of Porcine Heart

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The mechanical behavior of myocardial tissues plays a pivotal role in understanding cardiac function and dysfunction. In this study, we investigate the viscoelastic properties of two distinct regions of the porcine heart: the left ventricular myocardium and the septal myocardium. Utilizing advanced viscoelastic modeling techniques, we aim to characterize and compare the time-dependent mechanical responses of these critical cardiac tissues. Experimental data were acquired through Biaxial tests performed on tissue specimens extracted from the left ventricular and septal regions of the porcine heart. The viscoelastic models employed in this study encompass a range of constitutive equations, allowing us to capture the intricate behavior of the tissues under various loading conditions. Our findings provide valuable insights into the viscoelastic properties of the left ventricular and septal myocardia, shedding light on their distinct mechanical characteristics. Understanding these properties is crucial for advancing our knowledge of cardiac biomechanics and may have implications for the development of computational models, medical interventions, and therapies related to cardiac diseases and disorders. Overall, this study contributes to the growing body of research aimed at unraveling the complex mechanical behavior of cardiac tissues and enhances our ability to model and analyze the dynamic behavior of the heart, ultimately benefiting both clinical and research applications in cardiology and biomechanics.

Viscoelastic Characterization of Human Adipose Tissue Using Fung's Quasi-Linear Viscoelastic

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Fung's Quasi-Linear Viscoelastic (QLV) theory has been a cornerstone in modeling the viscoelastic tensile response of biological tissues for decades. This theory, deeply rooted in strain-history-dependent stress and fading memory principles, offers a comprehensive representation of relaxation behavior by incorporating a continuous spectrum of relaxation times. Within the framework of this one-dimensional theory, Fung's approach predicts key characteristics of soft biomaterials, such as relaxation, creep, stress insensitivity, and hysteresis to strain rate properties, making it a valuable tool for researchers. Furthermore, its simplicity allows for the extraction of essential material functions through relatively straightforward experiments, contributing to its widespread application and validation across various materials. In this study, we delve into the realm of viscoelastic mechanics to explore the mechanical properties of human adipose tissue. Uniaxial compression stress relaxation tests were conducted using adipose tissue samples obtained from the human abdominal region. The experimental data was fitted to a viscoelastic model, specifically, a quasi-linear viscoelastic (QLV) model. To characterize the elastic response, four different hyperelastic strain energy density functions were employed: a 5-terms polynomial function, a first-order Ogden function, an isotropic Gasser-Ogden-Holzapfel function, and a combination of a neo-Hookean and an exponential function. Among these models, the Ogden function emerged as the most suitable to describe the experimental data, highlighting its potential as a valuable tool for characterizing the viscoelastic behavior of human adipose tissue. The viscoelastic properties determined in this study are particularly crucial in relaxation tests conducted under finite strain rates. These properties help derive the long-term behavior of adipose tissue, which becomes especially relevant when estimating the static deformed shape of the tissue as time tends to infinity. Comparisons were made between the stiffness obtained in this study and previously reported results from the literature for adipose tissue sampled from different regions

of the body. These comparisons revealed a wide dispersion in the mechanical properties of adipose tissue across various studies, underscoring the importance of location-specific characterizations. Such variations may arise from factors like anatomical site, patient demographics, and experimental conditions, all of which can influence the viscoelastic response of adipose tissue. In conclusion, this work contributes to the growing body of knowledge regarding the viscoelastic properties of human adipose tissue. Leveraging Fung's Quasi-Linear Viscoelastic theory and employing the Ogden function, we have successfully characterized the elastic response of adipose tissue under compression stress relaxation tests. This information is invaluable for applications in the field of tissue biomechanics and can aid in the development of more accurate computational models for medical simulations, surgical procedures, and cosmetic interventions involving adipose tissue. However, the wide dispersion in mechanical properties underscores the need for further investigations, taking into account the various factors that influence adipose tissue behavior across different anatomical regions and patient populations.

Reduced order modelling and biochemical population-specificity in a computational model of cerebral aneurysm thrombosis: towards clinical applicability

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Computational fluid dynamics (CFD) models of cerebral aneurysm thrombosis are patient-specific insofar as geometry and haemodynamics are concerned. The biochemical reactions that result in clotting require considerable resources to fit all parameters on a per patient or population basis. Furthermore, translation of these CFD models to clinical contexts is limited by model complexity and computational cost. In this study, we present a model that couples results from a calibrated automated thrombogram (CAT), an in vitro test that is used to determine clotting function on a per patient basis, with CFD. The CAT data was fitted to population-specific biochemical profiles of haemophiliac, healthy and thrombotic patients, and applied to the aneurysmal wall of a 2D idealized geometry. There was faster clot growth in the thrombotic case, followed by the normal and haemophiliac cases, respectively. Complex vorticial structures formed as the different clots evolved. The patterns in clot growth, distribution of thrombin and fibrin, and velocity profile showed that there is a strong link between haemodynamics and biochemistry. The model was verified by comparing it to experimental results and it successfully captured the qualitative features of in vitro clotting. Polynomial and logistic regression machine learning algorithms were used to develop a reduced order model from CFD results. This model is relatively simple but would have far greater utility in a clinical context as it does not require solution of numerical methods or specialized CFD training.

Uniting auxeticity with extreme strength and high stiffness - the microstructure of limpet teeth

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Materials exhibiting a negative Poisson's ratio, which is also known as auxeticity, have been identified in both natural and engineered contexts, achieved through a variety of structural mechanisms. However, these typically adopt designs with lower stiffness due to the necessity of accommodating structural unit rotation or folding within available space. Consequently, the challenge of integrating auxeticity with high strength and stiffness has persisted. Our work explores the mechanical properties of limpet teeth, a material that performs remarkably well under demanding loading conditions. By employing in-situ nanomechanical testing within SEM and TEM, coupled with detailed investigations of its high-resolution structure and microstructure-based modeling, we unveil how the leading part of limpet teeth successfully attains this exceptional blend of properties.

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A multiscale and multiphase digical twin of function-perfusion processes in the human liver

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As the key organ for metabolic processes in the human body, the human liver is responsible for essential processes like fat storage or the detoxification [1]. To better understand the interplay between hepatic perfusion, metabolism and tissue in the hierarchically organized liver structure, we have developed a multicomponent, poro-elastic multiphasic and multiscale function-perfusion model, cf. [2], using a multicomponent mixture theory based on the Theory of Porous Media. The multiscale approach considers the different functional units of the liver, the so-called liver lobules, with an anisotropic blood flow via the sinusoids (slender capillaries between the periportal field and the central vein), and the hepatocytes, where the biochemical metabolic reactions take place. On the lobular scale, we consider a tetra-phasic body, composed of a porous solid structure representing healthy tissue, a liquid phase describing the blood, and two solid phases with the ability of growth and depletion representing the fat tissue and the tumor tissue. To describe the metabolic processes as well as the production, utilization and storage of the metabolites on the cellular scale, a bi-scale PDE-ODE approach with embedded coupled ordinary differential equations (ODE) is used. In order to represent realistic conditions of the liver, experimentally or clinically obtained data such as changes in perfusion, material parameters or tissue morphology and geometry are integrated as initial boundary conditions or used for parametrization and validation [3]. Data integration approaches like machine learning are developed for the identification, processing and integration of data. A workflow is designed that directly prepares the model for clinical application by (semi-) automatically processing the data, considering uncertainties, and reducing computation time.Enter your abstract here. Max. 500 words to fit on one page.

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2. Computation Modelling Biological Soft Tissues

Continuum kinematics-inspired peridynamics in Julia: A computational perspective

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Continuum kinematics-inspired peridynamics (CPD) is a peridynamic (PD) formulation that uses the same kinematic measures as classical continuum mechanics (CCM), providing a geometrically exact formulation [2]. PD is a non-local continuum formulation, wherein the behaviour of each material point is influenced by material points within a finite neighbourhood of that point [3]. By incorporating non-locality as a fundamental modelling concept, the range of interactions considered at each point is expanded, encompassing influences beyond its immediate neighbours. Simultaneously, the integral formulation simplifies the representation of spatial discontinuities by eliminating the need for explicit spatial gradient computations, making it highly suitable for modelling the intricate and heterogeneous nature of biological tissues. The implementation emphasises the complexities associated with incompressibility in material modelling. This contribution focuses on the implementation of CPD in Julia [1]. Several key aspects render Julia an ideal choice for the implementation of CPD. Julia is renowned for its computational performance, underpinned by its just-in-time compilation that allows for the efficient execution of numerical simulations [1]. Julia's performance-oriented design is well-suited for implementing and executing complex simulations efficiently. Julia has built-in support for parallel computing which empowers researchers to harness the full potential of multi-core processors and distributed computing environments. This capability proves invaluable, especially for large-scale simulations, where parallelization can lead to substantial acceleration in computational tasks. Additionally, Julia seamlessly connects with external libraries, simplifying the integration of existing numerical tools. The implementation of CPD in Julia offers a robust and powerful tool for simulating the intricate behaviour of materials where non-local effects are important, as well as in the presence of discontinuities. This work not only contributes to advancing the capabilities of PD simulations but also demonstrates the synergy between innovative computational frameworks and high-performance programming languages like Julia in tackling complex engineering and scientific challenges.

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Mechanomyography – a paradigm shift for investigating functional aspects of active biological tissue

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Muscles keep the human body functioning. Breathing, blood flow, digestion, posture, and movement depend on the interplay of neural signals and muscle tissues. Measuring neural signals that control, for example, motor units (MUs), the individual functional units of skeletal muscles, will enable over the next decades scientific breakthroughs in diagnostics and treatment, including the early detection of neurodegenerative diseases, optimizing personalized treatment or gene therapy, and assistive technologies like neuroprosthesis or exoskeletons control. In the field of skeletal muscle mechanics, all existing technology currently focuses on studying the neuromuscular system by measuring and processing the muscle's electric potential induced by the flow of ions across a skeletal muscle fiber's membrane and its link to force production. The methodology to record the resulting electrical field is electromyography (EMG). This technique is limited in its sophistication by fundamental physical restraints, i.e., smearing out of the signal as it propagates through biological tissues. This makes the localization and separation of the respective electrical charges an extremely challenging task. Hence, understanding muscle mechanics is subject to errors. The flow of ions, however, does not only result in an electrical field, but it also induces a magnetic one. Hence, in analogy of electromyography, one can utilize magentomyography (MMG) to gain information on the functional behavior of active skeletal muscle tissue by recording the respective magnetic field. Measuring the magnetic field, however, requires highly sensitive magnetometers – the emerging technology of quantum sensors. First proof-of-concept studies, including our in-silico studies, show that investigating the magnetic field is highly promising, in particular if a high-density magneto-myographic, or in short HD-MMG, setup is utilized. Using MMG to analyze the chemo-electromechanical behavior of skeletal muscles is a wide open topic that needs to be tackled and explored in the next decade(s). It is believed that this technology, in particular a HD-MMG setup, is superior to HD-EMG, in particular with respect to source localization and separation and will significantly enhance our understanding of muscle mechanics. This advantage will also be the enabler for imaging or determining morpho-functional characteristics. Such data, combined with the advanced computational musculoskeletal system models, will lead to a paradigm shift in analyzing muscle function.

Cell-Based blood flow modelling with HEMOCELL

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To investigate details of transport of platelets in e.g. the early phases of thrombosis, to appreciate the emergence of cell free layers in complex blood flow geometries and margination of platelets into these cell free layers, or to understand the flow of individual red blood cells in the microcirculation requires cell based blood flow modelling. Over the last decade we have developed a fully validated versatile suspension simulation environment, modelling millions of individual red blood cells and platelets, where the cells are modelled using a discrete element method, coupled to a Lattice Boltzmann model for the fluid phase using the immersed boundary method. [1] The fully parallelized code called HEMOCELL is available in the public domain (**https://hemocell.eu**). We report on some recent applications of cell-based blood flow modelling, in relation to hemostasis in punctured vessels [2] and effects of stiffened (diabetic) red blood cells, [3] as well as new applications in relation to aggregation of platelets in high shear environments. We will also discuss underlying computational requirements and report on parallel performance of the HEMOCELL code and recent developments in relation to domain decomposition and load balancing, and demonstrate behavior on large massively parallel production machines. Finally, we will discuss new avenues for our cell based modelling, in relation to coupling cell based modelling to continuous blood flow methods, where the cell based model informs the continuous flow model on quantities such as e.g. shear induced diffusivity of platelets, and in relation to new applications in thrombosis modelling and in the microcirculation in the brain.

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The Cerebrovascular System in the Virtual Human Twin

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Our aim is to deliver validated multi-scale computational models for improved treatment and fundamental understanding of acute strokes, both ischemic and hemorrhagic, and demonstrate added benefit of these models for personalised disease management. To this end we develop validated, integrated multi-scale, multi-organ models for cerebral blood / Cerebral Spinal Fluid, brain perfusion and metabolism, and blood flow and thrombosis along the heart-brain axis, by integrating available and newly developed dynamic, interoperable, and modular computational models. Here we report on integrated 1D/0D blood flow models for flow from the heart to the major cerebral arteries and from there to the brain surface, and coupled to full blown three-dimensional coarse-grained models for brain perfusion. We demonstrate how to include the leptomeningeal collateral circulation, a very relevant collateral circuit for patients suffering acute ischemic stroke. The perfusion model is coupled to a brain metabolism model, to capture infarction of brain tissue after a stroke event. Finally, we report on applying the model for the Cerebrovascular system to acute ischemic stroke. [1] A stroke event is mimicked by blocking one of the major cerebral arteries. A drop of perfusion in the brain territory that is fed by the blocked artery is observed. Next, infarction is modelled, and the resulting volume of infarcted tissue is measured. Our results are compared to retrospective clinical data from the Mr. Clean trial, demonstrating that on the population level our stroke model is capable of reproducing results from the Mr. Clean trial. As next steps, and as part of the EU-funded Gemini project, [2] we will add additional models for cerebral aneurysms, hemorrhagic strokes, vasospasm, and oedemas. We will fully personalize specific models for acute ischemic strokes and in a clinical trial prove added value of applying such model as decision support in treatment of acute ischemic stroke.

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Patient-specific Finite Element Study of the Cardiac Biomechanics in Peripartum Cardiomyopathy

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Peripartum cardiomyopathy (PPCM) is an idiopathic cardiomyopathy in the last month of pregnancy or after delivery. PPCM is associated with high mortality (8.0-9.8%) and diagnosed by exclusion [1]. The current study aimed to investigate the cardiac biomechanics in PPCM using patient-specific finite element (FE) models to identify characteristics suitable for improved and differential diagnosis. Three-dimensional biventricular geometries were reconstructed from magnetic resonance images of six PPCM patients with different disease severity. FE models coupled to a lumped-parameter circulatory system were developed in Abaqus [2]. Myocardial fibre orientation was implemented using a rule-based method. Passive and active material properties defined in the constitutive formulation of the myocardium were optimized for each patient [2]. The PPCM FE models accurately predicted the patient-specific clinical left ventricular (LV) ejection fraction (23% ± 15%) and stroke volume (35 ± 15 ml). The myocardial contractility was $Tmax$ = 170 ± 45 kPa. The circumferential strain was considerably greater in the LV than the right ventricle (RV), i.e., -13.2% ± 9.33% versus -6.93% ± 4.37% (p = 0.056), whereas the longitudinal strain was considerably greater in the RV than the LV, -7.55% ± 5.02% versus -2.78% ± 2.86%, (p = 0.055). The myofiber stress was two-fold higher in the LV (30.4 ± 10.9 kPa) than the RV (14.6 ± 3.9 kPa, p = 0.03) at end-systole but similar in the LV (6.1 ± 2.0 kPa) and RV at end-diastole (5.6 ± 1.8 kPa, p = 1.55). In PPCM, LV longitudinal strain was lower than, but circumferential strain was similar to those reported for the healthy case. Myocardial contractility and LV myofibre stress were higher in PPCM than in the healthy heart but similar to heart failure. The current results offer limited diagnostic value. However, the developed patient-specific cardiac models provide the basis to further study the pathological cardiac biomechanics associated with PPCM to aid in the development of novel diagnostic approaches.

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Investigations of hyperelastic constitute models of healthy and cancerous breast cells at various strain rates

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Cancer is a major public health burden in South Africa and other developing countries. The incidence of cancer around the world has been increasing steadily. With the advances in micro-and nanofabrication technologies, it has been possible to investigate the mechanical properties of a single cell. In this study, we investigated the stress analysis of healthy (non-malignant MCF10A) and cancerous (malignant MDA-M001B-23) breast cells. A nonlinear elastic finite element method was employed to simulate Ogden constituted model. The study was carried out at 20%, 30%, and 40% compression of a healthy and cancerous cell. The accuracy of mechanical properties depends on how long the model will last at a certain time. As such, the strain rate of the cell was selected as 0.03, 0.1, and 0.5. Then the maximum compression force of 600pN was achieved when 30% - 40%, which was similar to the experimental data. During the 40% compression, the cancerous cell cytoplasm was not able to withstand the applied load and the maximum stress of 1.349e-2 Pa was reported. These results demonstrate that the healthy cell is stiffer than the cancerous cells.

Biomechanical simulation of the brain using a meshed anatomical atlas

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Computational methods such as the finite element method are commonly used to predict brain deformations in areas ranging from neurosurgical planning to impact injury simulations. Analyzing brain deformations can provide critical insights into brain shifts, enhancing the precision of neurosurgical planning, as well as quantifying the severity of trauma in incidents such as vehicle accidents or sports injuries. A significant limitation, however, lies in the capacity to visualize and analyze these computed brain deformations against the anatomical structures of the brain. Understanding the brain's anatomy offers critical insights regarding the complex functionality and precise spatial locations of the different parts within the brain. The link between the computed deformation resulting from computational simulations and the brain's anatomy is currently lacking, primarily due to the complexities of accurately recovering distinct anatomical structures of the brain from existing scanning technologies. To address this limitation and enable comprehensive biomechanical brain simulations, we present a meshed anatomical atlas. Our method establishes a two-way correspondence between the anatomical brain structures and the computational grid used for simulating brain deformations. This method involves the use of an open-source digital brain atlas, effectively bridging the gap between detailed anatomical information, finite element mesh and computational results and corresponding predictions. We use the Open Anatomy's SPL/NAC Brain Atlas, which details over 300 anatomical structures of the brain and is freely available to the public [1]. This study demonstrates the utility of our approach using a case study of electrode placement-induced brain shift. Specifically, we simulated a common neurosurgical procedure used to identify the epileptic seizure onset zone, by predicting the brain shift caused by the implantation of a subcortical electrode grid [2].

After solving the biomechanical model, we extracted and analyzed displacement statistics relative to various anatomical structures within the brain. This approach reveals the relationship between electrode placement and localized anatomical responses. This study constitutes the first step towards integrating an open atlas and FE simulations to achieve highly detailed, anatomically based analyses and visualization of results. We hope to extend our research by applying this approach to subject-specific and/or patient-specific cases in the future.

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Bi-ventricular Elastic Material Parameters Estimation Using 3D CMR Strains in RHD Patients

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Insight into the biomechanical properties of myocardial material behavior in healthy and diseased hearts using finite element analysis could provide important information on cardiac function and potential treatment of the diastolic abnormalities responsible for ventricular hypertrophy and inflammation. To ensure a realistic myocardial constitutive behavior, inverse modeling based on the finite element approach combined with the Levenberg-Marquardt method is used for the material parameter optimization. The end-diastolic pressure-volume relationship (EDPVR) and strains were used to estimate the elastic material characteristics. Global circumferential-, longitudinal-, and radial strains were considered, and corresponding different multi-objective optimization problems were designed. Here we report on the sensitivity of elastic material parameters and muscle fiber orientation angles regarding the specific strain components included as targets in the objective function. Patient-specific computer simulations of EDPVR and strains for all objective functions showed good agreement with clinical data. The difference between the predicted and clinical parameters is less than 0.1%. We present qualitative and quantitative differences in stress and strain distributions for each of these optimization experiments. Model calibration utilizing EDPVR and strain could result in more accurate elastic material properties.

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3. Inverse Problems, Optimization and Design

Interpretable Latent Spaces of Rail-Guided Wave Spectrograms using Independent Component Analysis and the Latent Space Perspicacity and Interpretation Enhancement Framework

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This study presents a data-driven approach to enhance the interpretability of latent representations for a Guided Wave Ultrasound (GWU) based monitoring system installed on railway track. The railway track infrastructure requires condition-based maintenance to ensure safety and prevent severe derailments caused by defects like cracks. The monoting system relies on the propagation of guided waves in the rail to detect defects and have been shown to be effective in detecting defects at long ranges, with distances of up to 2km between the transmitter and receiver stations [1]. We investigate the applicability of Independent Component Analysis (ICA), and the clustering and ranking of latent vectors to learn interpretable latent representations from the spectrograms, which represent time signals captured by the monitorring system as time-frequency spectrograms using the Short-Time Fourier Transform. The model is trained in a supervised manner using simulated data and tested on experimental measurements, enabling the separation and transformation of signal components based on statistical independence. Simulated spectrograms are generated for training and testing purposes, and noise is introduced to prevent overfitting. This approach allows for fine-tuning input and output parameters, enabling the extraction of essential features from the reduced latent space. The employed framework automates the clustering and ranking of latent vectors to enhance the interpretation of latent vectors from the ICA model . The framework allows for ranking latent directions, scaling of latent directions, and automatic clustering of latent directions into a specified number of clusters, and we are able to automatically determine the appropriate number of clusters to condense the latent directions. This approach improves the interpretability of underlying variables in both simulated and field-measured spectrograms, ultimately enhancing the effectiveness of interpreting railway track monitoring measurements using the GWU-based system.

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A Framework for the Design of Soft Pneumatic Actuators Using Computational Tools

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Soft robots possess significant potential in applications such as human-to-machine interfaces and delicate handling operations. Unfortunately, their development is hindered by the complex design space resulting from nonlinear material behaviour. This makes finite element simulations costly and difficult to interpret. This study utilizes a hierarchical design approach to create soft pneumatic actuating units by combining designer intuition with computational tools. Our approach integrates Physics Engines, Finite Element Analysis, Metamodeling, Optimization, and parallel computing, orchestrating a process to efficiently design soft pneumatic actuators. The main goal is to create a replicating unit that can be assembled into a soft robot. Such a replicating unit has been previously developed in the Evogym Benchmark developed by researchers at Massachusetts Institute of Technology (MIT). The designed units follow idealised deformations and the unit was not realised. We demonstrate real-world deformations achieved through the shape, placement, and interplay of pressurized and unpressurised cavities, controlling the deformation process. This pneumatic setup enables pressurized cavities to create deformation while unpressurised cavities absorb deformation. A variable stiffness effect is achieved using this setup. Together these features allow for achieving complex deformation. Our process achieves realistic models that closely match the idealized models used in the Evogym Benchmark. This process creates a crucial link between cost-effective physics environments and the practical realization of the actuators. Our approach is versatile and holds great promise for advancing soft robotics through pneumatic actuation.

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4. Manufacturing and Process Engineering

Evaluation of the stress distribution on the polyurethane trileaflet heart valve leaflets in the closed-to-open configuration

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Developing an affordable prosthetic valve for the 33 million people with rheumatic heart valve disease who are younger than 65 is an issue facing sub-Saharan Africa and the developing world [1]. It is costly and time-consuming to design and manufacture functional polyurethane heart valve prototypes, to evaluate and comprehend their hydrodynamic behaviour [2]. To rapidly enhance heart valve replacement designs, to meet the minimal criteria of FDA and ISO regulations and specifications and to reduce the requirement for lengthy clinical testing, computational fluid dynamics (CFD) and finite element analysis (FEA) were used. In this study, the stress distribution on the leaflets of a polyurethane trileaflet heart valve in the closed-to-open configuration was analysed using FEA. The geometry of the valve from an earlier prototype was improved. In addition, the leaflet thickness, coaptation and free edge areas, as well as the height and flexibility of the stent, were examined as design criteria. An improved method to compare valve performance is to use its geometric orifice area (GOA) rather than its average pressure drop, as the latter does not indicate how well the mass flow rate through the valve is performing.

The results revealed that when the flexibility of the stent was taken into consideration with a uniform leaflet thickness, stress concentration regions that were present close to the commissural attachment were greatly diminished. Furthermore, it was found that the stress on the leaflets was directly impacted by the effect of reducing the post height on both rigid and flexible stents. When the flexibility of the stent was considered, a varying leaflet thickness close to the commissures did not appear to reduce the leaflets stresses. The free edge geometry was shown to directly affect the GOA and, in turn, the valve's closing fluid volume. An investigation into how calcification due to high stresses might affect the structural integrity of polyurethane leaflets, is still to be done.

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Digital Fabrication for pierced vault: Hole percentage vs instability behavior

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The growing focus on masonry and non-metallic constructions demonstrated their ongoing potential as cutting-edge engineering and architectural solutions. The form finding procedure for a cement-based, tessellated, pierced vault is implemented in this study. The ideal design for a compression-only vault was determined using the multi-body rope approach (MRA). Rhino-vault was subsequently implemented by truss network analysis (TNA) for a further shape validation and for the definition of various surface tessellation meshes based on various hole pattern configurations. In order to identify the optimal solution, various vault piercing percentages were taken into consideration and compared. Furthermore, the geometry solutions were subjected to mean global stability analysis, accounting for the variations in hole placements. Furthermore, the geometry solutions were subjected to mean global stability analysis, accounting for the variations in hole placements. Additionally, a completely environmentally benign method of 3D printing using the Fuse Deposition Modeling (FDM) technology is investigated for the creation of formworks for cement-based blocks, or dowels, which are necessary for the assembly of a scaled prototype vault. The vault prototype, which had a specific piercing %, was put through several loading scenarios and monitored by a non-contact device using Digital Image Correlation (DIC) technique. beforehand. Measurements of displacement correlated with the various loading stages up to the point of collapse were performed.

Residual Stress Analysis of Outside Turning of Ti6Al4V Titanium at Varying Cutting Speeds with and without Coolant

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A numerical and experimental investigation was conducted to study the residual stresses induced by the outside turning of Ti6Al4V titanium. The study examined different cutting speeds, ranging from 30 to 200 m/min, with and without a coolant. Surface XRD and the incremental hole-drilling strain gauge method were used for experimental measurements of in-plane residual stresses. Additionally, a 2D thermal-mechanical coupled finite element method (FEM) model was developed for numerical simulations. The prediction of tool wear and its impact on residual stresses were considered, with worn tool insert profiles used as initial states for the simulations. A numerical and experimental investigation was conducted to study the residual stresses induced by the external turning of Ti6Al4V titanium. The study considered several cutting speeds ranging from 30 to 200 m/min, with a 0.2 mm/rev feed rate. The experiments involved surface X-ray diffraction and incremental hole drilling strain gauge methods to measure in-plane residual stresses. A 2D thermal-mechanical coupled finite element method (FEM) model was also developed for numerical analysis. The prediction of tool wear and its impact on residual stresses were also considered. A study investigated residual stresses induced by outside turning of Ti6Al4V titanium at various cutting speeds with and without a coolant. Cutting speeds ranged from 30 to 200 m/min, a feed rate of 0.2 mm/rev was used for all tests. X-ray diffraction and incremental hole-drilling strain gauge methods were employed for experimental measurements of in-plane residual stresses on the machined surface and their depth variations. Furthermore, a 2D thermal-mechanical coupled finite element method (FEM) model was developed to predict tool wear and analyse residual stresses at different depths for initial and worn tool conditions. This study investigated the residual stresses induced by the outside turning of Ti6Al4V titanium at various cutting speeds with and without a coolant. The experimental work involved surface XRD and incremental hole-drilling strain gauge method to measure residual stresses in the plane. Additionally, numerical work was conducted using a 2D thermal-mechanical coupled finite element method (FEM) model. Tool wear prediction was initially considered for a cutting length of 30 mm at each speed, followed by analysing residual stresses versus depth for both the first cut pass and the two passes of a worn tool insert.

Review on the Effect of Heat Treatment on Microstructure and Mechanical Properties of Metallics

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There is a high need for parts with well-balanced mechanical properties in industries. This is achieved through the use of various heat treatment processes. The adjustment of heat treatment parameters can lead to a diversity of microstructures. The heat treatment parameters of cooling, such as furnace, air, oil, and water cooling, as well as the soaking time, play important roles in determining the characteristics of microstructures obtained. The importance of this is underscored by the fact that the mechanical properties of metallics, such as strength and ductility are dependent on their microstructures. This paper presents a review of the effects of annealing, normalising and high temperature annealing heat treatments on the microstructures and mechanical properties of Ti6Al4V, high-strength steels and aluminium alloys. It is clear from this study that, annealing coarsens the microstructural features, reduces hardness and strength, and increases ductility and machinability of all three different alloys considered here, while normalising refines their microstructures and improves strength, while ductility is reduced. Evidently, heat treatment processes play an important role on the microstructure and mechanical properties of the three alloys. Therefore, structural parts with well-balanced mechanical properties needed in various industries can be achieved through the applications of these heat treatment processes.

5. Material Design and Modelling

Multiscale Coupled Phase-Field Model for Prediction of Mechanical Property Evolution

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Embrittlement due to thermal exposure results in reduced ductility of metal alloys. This significantly impacts the loss of design function of industrial installations. The cause is directly attributed to the microstructural evolution governed by the thermodynamic and kinetic properties of the alloying elements. The phase-field method is a robust technique for modelling microstructure evolution, recognised for its ability to simulate complex geometries and integrate thermodynamic and kinetic data. It uses a diffuse-interface, eliminating the need to track interfaces during microstructure evolution, and allows for the prediction of complex grain morphologies. The method uses differential equations to represent time-dependent changes in phase-field variables, which are solved numerically. It can incorporate various driving forces for microstructural evolution, such as decreases in bulk, interfacial and elastic energies. However, it is phenomenological and does not directly address the behaviour of individual atoms. Material-specific properties are included in the model through phenomenological parameters, determined based on experimental and theoretical data [1]. Coupling the phase-field model with a mechanical model would provide a holistic view of changes in macro properties. The study focuses on duplex stainless-steel grade 2205, a low-carbon alloy widely used in industrial applications. This material is prone to thermal embrittlement caused by spinodal decomposition and precipitations in the ferritic phase [2]. Microhardness tests were conducted on samples that were heat-treated at 500°C. This provided a time-based hardness profile (nonlinear) and a reference for model validation. The mechanical model is derived from an exponential curve fitting to the experimental profile to account for global changes, and Euler's formula to account for local perturbations. Both accounts produce parameters related to the material in particular, changes in volume fractions and the minimisation of the free energy. These parameters are obtained from the phase-field model and incorporated to account for the evolution. Challenges arise naturally due to the multiscale spatiotemporal differences between the two models. The difficulties were overcome by introducing dimensionless scaling variables, which also solved any inaccuracy of the material-specific data. The coupled model produced favourable results against the experimental data.

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Continuum-kinematics-inspired peridynamics: Transverse isotropy

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Peridynamics (PD) is a non-local continuum theory [1]. Continuum-kinematics-inspired peridynamics (CPD) is geometrically exact and utilizes non-local kinematic measures that are analogous to those from classical continuum mechanics (deformation gradient, its co-factor and Jacobian) to model realistic materials [2]. In CPD the interaction potential is decomposed into parts corresponding to one-neighbour interactions, two-neighbour interactions, and three-neighbour interactions. The one-neighbour interactions of CPD are identical to the interactions of the original bond-based PD. This work focusses on capturing transverse isotropy in the CPD framework. A general format of the interaction energy double-density that satisfies the representation theorem will be presented [3]. Through a series of examples, we will demonstrate how this format can be utilised to recover transverse isotropic peridynamic formulations found in literature. We will compare the material responses of these (and other) formulations for a body subjected to large deformations. Lastly, transverse isotropic formulations unique to CPD will be showcased.

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Investigating the Effectiveness of three mixing Techniques by Quantifying Dispersion and Homogeneity of CNTs/Ti6Al4V(ELI) powder mixtures using Image Analysis

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Homogenous dispersion of carbon nanotubes (CNTs) is difficult to achieve because they aggregate into bundles due to the highly attractive Van der Waals forces which result in their poor dispersion in a matrix. The energy required to effectively disperse CNTs must be sufficiently high to overcome the Van der Waals forces, however, not so high to cause damage to them. Three methods of mixing were investigated using image analysis of scanning electron microscope (SEM) images of powder mixtures. Existing methods of dispersion are subjective to data and the materials of the mixture and require cumbersome mathematical approaches. Therefore, in the present work a statistical approach, accompanied by image analysis was carried out to quantify the effectiveness of the three methods of mixing in dispersing CNTs in Ti6Al4V(ELI) at 3% and 8% vol%. of CNTs. The loss of reinforcement due to agglomeration was determined by comparing the total perimeter of the longitudinal sections of the calculated number of CNTs contained in a given surface area of a CNT agglomerate in a scan, with its perimeter. Several methods including sonication, surfactant, and high-speed rotators are used to achieve the dispersion of CNTs in Ti6Al4V(ELI). A major obstacle to such efforts is that CNTs aggregate into bundles because of highly attractive van der Waals (vdW) forces in them, thus causing poor dispersion of CNTs within most aqueous media. Mechanical agitation by ultrasonication produces temporary dispersion of CNTs in aqueous media, however, it is often subsequently followed by

agglomeration of the dispersed CNTs. Three methods of mixing were considered including mechanical, tubular, and combined mixing. The results from the experimental study showed that combined mixing was more effective in dispersing CNTs in a Ti6Al4V(ELI) matrix, due to the formation of agglomerates with smaller areas and perimeters than the other two methods of mixing. The results from the research showed that a loss in reinforcement would occur in mechanical mixing and tubular mixing as these two were the least effective methods for dispersion. Large sized agglomerates were found in mechanical mixing and tubular mixing compared to the combined mixing method. It is therefore expected that reinforcement would be less effective in these two mixing methods.

Computational micromechanics modelling to establish a Process-Structure-Property relationship for additively manufactured 316L Stainless Steel struts

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Metal additive manufacturing (AM) is revolutionizing manufacturing industry through the utilization of a layer-by-layer building process that allows highly complex, bespoke and customized component designs to be produced accurately and efficiently. Laser powder bed fusion (LPBF) is one such AM technique that is gaining popularity as a versatile and time-efficient method for manufacturing intricate parts directly from CAD designs, especially for biomedical applications such as stents or patient-specific orthopaedic implants [1]. However, the microstructures resulting from metal AM processes, including grain morphology, crystallographic textures, and defect distributions, are very different to those generated by conventional manufacturing processes. Therefore, there is a critical need to investigate the effects of such microstructures on the mechanical performance of AM-generated components. This is particularly the case for very small components, such as stents, scaffolds and filters, that are widely used in biomedical applications, and that are typically composed of thin metallic struts (< 100 μm). Here we consider AISI 316L stainless steel, given its widespread use in medical device applications, and especially in coronary stents. The work is focused on the development of a process-structure-property (PSP) relationship for thin AM-generated 316L struts, through detailed computational micromechanics modelling. For the process-structure (PS) aspect, geometrically based methods [2] and cellular automaton (CA) methods are utilized to generate representative strut microstructural geometries, including explicit representation of grains, texture and defects, as a function of AM process variables (hatch spacing, layer thickness and laser energy density). For the structure-property (SP) aspect, these microstructures are incorporated into detailed crystal plasticity finite element (CPFE) strut models [2] to predict mechanical properties (ductility, yield strength and UTS). The combination of the two aspects establishes a complete PSP relationship for the struts, relating the AM process variables to the mechanical properties. This methodology has allowed for the identification of optimal AM process variables (hatch spacing and layer thickness) to result in desirable mechanical properties (ductility and strength) with high manufacturing efficiency (low laser energy density).

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Development and preliminary numerical investigations of a dislocation density-based finite-strain rate-dependent elastoplasticity constitutive model

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Finite-strain elastoplasticity constitutive models suitable for process-scale simulation are typically developed from empirical observations of phenomena of interest. Such models make use of internal state variables that do not directly represent the associated evolution of the material microstructure, such as accumulated plastic strain. As a result, these models cannot directly provide microstructural information that may be of interest. In an attempt to bridge this gap, a mechanistically-motivated, three-dimensional, finite-strain, rate-dependent elastoplasticity constitutive model is developed in this work by using dislocation density as an internal state variable that evolves according to the Kocks-Mecking model. The behaviour of the model is elucidated after numerical implementation and computational experiments with several loading cases, such as cyclical loading, uniaxial compression, plane strain compression, and stress relaxation. In contrast to other dislocation-based rate-dependent elastoplasticity models, the model presented in this work is formulated in a finite-strain setting that is suitable for the macro-scale simulation of wrought metal production processes.

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Exascale Materials Calculations From First-Principles

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The creation of robust, adaptive software and algorithms that can fully exploit exascale capabilities and future computing architectures is critical to designing advanced materials and devices with targeted properties. We have developed an open-source code that discretizes the density-functional-theory equations on real-space grids that are distributed over the nodes of a massively parallel system via domain decomposition. Multigrid techniques are used to greatly accelerate convergence while only requiring nearest neighbor communications, while a novel adaptive finite differencing scheme dramatically improves accuracy. The real-space multigrid (RMG) code achieves the same average accuracy as plane wave codes on the well-known Delta test for 71 elements in the periodic table and can handle all Bravais lattice types. It scales from desktops and clusters to supercomputers, including the exascale Frontier and pre-exascale Summit and Perlmutter systems, while utilizing all CPU cores and GPUs in each node. RMG is distributed via www.rmgdft.org, with over 4,000 downloads to date. Due to its computational efficiency, RMG is very suitable for large-scale survey approaches, including Materials-Genome and Machine-Learning projects.

In collaboration with E. L. Briggs and W. Lu.

Central Pattern Generator for Pneumatic Soft Robots

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Soft robots open many possibilities to embed intelligence within the structure of a robot. However, central control of external valves and many control lines typify pneumatic soft robots. This study proposes a soft pneumatic pattern generator to control two pneumatic actuators' activation simultaneously. The concept mimics biological locomotive control, where nerve clusters distributed throughout the body control the activation of muscle fibres rather than a central brain. The brain sends relatively simple proportional signals, converted to more intricate patterns locally. Adapting this concept to soft robotics simplifies their typical control requirements. The proposed pattern generator controls two actuators connected to a single pressure supply. Each actuator articulates out of phase with the other. The pressure curves are similar for each output, producing a balanced oscillation of the two actuators. Increasing the supply pressure increases the frequency of oscillation. This configuration better controls symmetric, biomimetic locomotors than previous realisable pneumatic central pattern generators.

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6. Multi-scale and Multi-physical Problems

Computational mechanics of light responsive elastomers: from coupled multi-physics problems to soft robotics applications

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Liquid crystal elastomers (LCEs) are polymeric materials that undergo large deformation in response to a large variety of external stimuli (heat, light, electro-magnetic fields). For this reason, they are receiving increasing attention as responsive materials for robotic applications. Here, thanks to their unique properties, LCEs can be exploited to conceive and engineer robotic systems that are multi-responsive, locomotive, interactive, capable of self-feedback and self-regulating [1].
Among the possible applications of LCEs, autonomous robotic micro-swimmers entirely powered by light provide a particularly interesting example [2]. In fact, LCEs provide us with an ideal playground for the development of multi-physics computational tools. Besides the fluid-structure interaction (FSI) necessary to resolve the motion of an autonomous swimmer, heat transfer, light propagation and absorption, steering by applied electric and magnetic fields need to be resolved simultaneously, and in a large deformation setting [3].
In this talk, which also draws on joint work with Alessandro Lucantonio (Aarhus University, Denmark), Reza Norouzikudiani (Scuola Superiore Santanna Pisa, Italy), and Luciano Teresi (Università RomaTRE, Italy), we will review recent efforts from our group to develop theoretical and computational models for the simulation of FSI problems for soft robots made of LCEs. We will discuss heat-powered artificial cilia capable of stirring a fluid in micro-fluidics applications and light-powered micro-swimmers for biomedical applications.
Partial support for this research has been provided by European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956150, project Storm-Bots (https://storm-bots.eu).

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Fully Coupled Thermo-Chemo-Mechanical Peridynamics

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Peridynamics (PD) is a powerful tool for addressing crack-related issues. However, existing general PD models do not adequately account for the coupling of multiple physical fields. This study introduces a novel PD model that effectively incorporates the coupling of deformation, heat conduction, species diffusion, and chemical reactions. First, the balance equations for mass, linear momentum, and energy are formulated. Subsequently, fully coupled constitutive relations are established to describe the interactions between these diverse physical quantities. These relations are then utilized to derive evolution equations governing the flow of species and heat from the energy dissipation inequality and chemical kinetics. Species diffusion and chemical reactions are treated as distinct processes to investigate their respective effects on the Helmholtz free energy density of solids, as well as their role in crack formation and propagation. Moreover, a calibration process is undertaken to align specific coupling coefficients with their counterparts in continuum mechanics. To validate the model, three specific cases are simulated: the redistribution of vacancies in ceramics, hydrogen trapping phenomena, and embrittlement in metallic materials.

Partitioned coupling of Euler-Bernoulli beams and incompressible viscous Newtonian fluids for fluid-structure interactions

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This paper assesses the ability of the open-source Computational Fluid Dynamics software TrioCFD [1] to solve fluid-structure interaction (FSI) problems. The software employs an Arbitrary Lagrange-Eulerian method to handle moving boundaries, allowing accurate representation of structural deformation within the fluid domain [2]. The high computational resources required for FSI simulations can be a limitation for industrial applications. To address this, a one-dimensional Euler-Bernoulli beam model is proposed as a simplified modeling approach for slender structures. The beam model is integrated into TrioCFD, enabling internal fluid-structure coupling and reducing data exchange between separate software. The time coupling is based on a classic explicit serial algorithm. The model is validated first through test cases involving two coaxial flexible and circular cylinders separated by a viscous Newtonian fluid at rest. The results, including fluid forces, added mass and damping, and various types of boundary conditions of the cylinders, are analyzed and compared to reference data [3]. The coupling algorithm is then challenged by adding both axial and cross fluid flow. The study highlights the potential of simplified modeling approaches for slender structures, such as the Euler-Bernoulli beam model, in reducing the computational resources required for FSI simulations, making them more accessible for industrial applications.

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A Macro-scale approach to Computational Fluid Dynamics Modelling of the Reduction of Iron and Manganese ore by Hydrogen

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The carbonaceous reduction of iron and manganese ores is an energy-intensive process that releases large amounts of pollutant gases. In an attempt to circumvent the greenhouse gas emissions, hydrogen is currently being investigated as an alternative reductant. The reduction of iron and manganese ores with hydrogen results in the structural changes in the intermediate products which might limit the diffusion of the reactant gases through the pores. Computational models that capture the structural changes and the resultant operating regime will describe the regime transition accurately and benefit the design of reduction reactors. The current work predicts the degree of reduction in a packed bed reactor under hydrogen reducing conditions. The iron and manganese ores are described as a collection of scalar and tensor fields such as thermal conductivity of the porous medium, density and viscous resistance.

Modelling polycrystalline agglomerates for intercalation batteries

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The research of new electrode materials such as sodium ion intercalation compounds is key to meet the challenges of future demands of sustainable energy storage. Many commercial as well as promising electrode materials exhibit strongly anisotropic properties and are synthesized as polycrystalline agglomerates. These two factors lead to a strong correlation between the hierarchical particle morphology and effective ion transport in the host material. Simultaneously, the microscale interactions of chemical, electrical, and mechanical forces determine the intercalation dynamics and, consequently, exert a substantial influence on overall cell performance. In the realm of computational simulations, a gap exists between the atomistic understanding of diffusion in a perfect crystal and the effective diffusivity of secondary particles, which is used in porous electrode theory. A suitable tool to bridge this gap by studying the anisotropic transport in polycrystalline battery materials, is the multiphase-field method. Our previous work [1] highlights the capability to simulate multi-grain battery materials in the micrometer range including phase transformations and heterogeneous nucleation at existing grain boundaries. Our investigations encompass a spectrum of secondary particle structures, ranging from those characterized by random grain orientations to highly textured specimens. The simulated ion distributions match qualitatively with experimental observations of transition metal valence states [2]. Furthermore, we show how these simulations can be used to mimic potentiostatic intermittent titration technique (PITT) measurements and compute effective diffusion coefficients for secondary particles, revealing the connection between particle microstructure and apparent diffusivity [3]. Consequently, the modeling framework can be employed to guide the microstructure design of secondary battery particles. In the bigger picture, simulations of polycrystalline agglomerates pave the way for a multi-scale investigation of battery materials from nano-sized single crystals to a porous electrode consisting of hierarchical secondary agglomerates. This holistic approach holds the potential to guide research towards batteries with longer lifetime and improved rate performance.

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High performance magnets for efficient energy conversion: A micromagnetic study

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Magnetic materials play a crucial role in improving the efficiency of conversion devices, including transformers, power generators such as wind turbines, sensors and electric motors used in electric mobility, cf. [1]. Their importance in enhancing operational performance for industrial applications has led to a growing research interest in high-performance magnetic materials. This interest focusses primarily on the reduction of environmentally critical substances, the improvement of performance, and the reduction of energy needed for the production. Simulations can support the design process of performance and resource optimized microstructures. Finite elements have proven to be strong in an exact approximation of heterogeneous microstructures, and the micromagnetic theory has emerged as a powerful tool for the accurate analysis of magnetic phenomena on micron scales, cf. [2]. Micromagnetism imposes a constant length on the magnetization vectors throughout the simulation, which is numerically a non-trivial task. This constraint is resolved via a perturbed and condensed Lagrange multiplier. This contribution, compares and analyzes the impacts of a severe plastic deformation based process route, on the production of magnets and its resulting effective properties, cf. [3]. Since the nature of this method is to subject materials to very strong plastic deformations, the focus remains on possibly induced imperfections, such as cracks and stresses, and their effects on the effective magnetic response behavior.
Nevertheless, other influences, such as those of secondary phases, are also considered.

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7. Numerical Simulation Methods

A comparative analysis of homogenisation techniques applied in numerical modelling of corrugated paperboard boxes

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Corrugated paperboard's overall behaviour is affected by the material properties of the individual paper sheets as well as the combined properties of the board. Numerical modelling of corrugated paperboard is quite challenging due to its waved geometry and material non-linearity. Because of the complex geometry and material behaviour of the board, there is still scope to enhance the accuracy of current modelling techniques as well as gain a better understanding of the structural performance of corrugated paperboard packaging for improved packaging design. A practical material characterisation method for full-scale box simulation that defines different material properties for the box edges/corners and panels and considers both linear and non-linear deformation of the board for full-scale box simulation is proposed in this study.

The study is divided into two parts. In the first part of the study, for full-scale box simulation, the finite element model is divided into different regions, the edges/corners (both horizontal and vertical corners) and the side panels of the box respectively. Each of these regions is described using different material properties. The box edges/corners are described using the optimal material properties from bending tests conducted on creased samples and edge compression tests, while the box panels are described using optimal material properties obtained from bending tests conducted on samples without creases.

To compare the results of the developed model that takes into account failure of the material around the corners. A finite element model of a full-scale box with the same material properties defined for the entire box is developed using the optimal material properties obtained from bending tests conducted on uncreased samples. The accuracy of these two approaches in predicting the deformation of the panel and the compression strength of the box is evaluated, and a practical material characterisation method for corrugated paperboard boxes is proposed.

Modelling Complex Ultrasonic Reverberations in Rail Track Inspections for Accuracy or Interpretability: A Review of Two Semi-Analytical Finite Element Based Methods

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The development of ultrasonic guided wave monitoring systems has become increasingly important due to their ability to detect damage in structures. These monitoring systems use piezoelectric transducers that are permanently attached to waveguides, such as rails and pipelines, to excite and receive ultrasonic guided wave signals. Changes in signals can provide a reliable indication of damage growth in the waveguide and ultimately reduce unwanted catastrophes. However, in the context of railway lines, obtaining monitoring data containing damage signatures is challenging as damaged sections of rail are immediately replaced when detected. Laboratory damage experiments are often infeasible due to end reflections from short sections of rail dominating the response. Therefore, modelling and simulation become increasingly important for simulating unavailable damage scenarios to help in the development of robust guided wave-based monitoring systems. To simulate reliable inspection signals, it is essential that the model employed accurately captures the physics of the problem and offers valuable insights into wave propagation and interaction. However, the complexity of wave propagation in a waveguide with multiple discontinuities, involving multiple modes and complex reverberations, makes it impossible for a single model to satisfy both requirements. Therefore, this study addresses this dual challenge by considering the complementary nature of two numerical approaches for accurate and interpretable simulations, respectively. The two approaches model and simulate guided wave inspections encompassing the excitation, propagation and scattering from discontinuities in 1D waveguides. The major contribution of these procedures lies in their ability to simulate complex back-and-forth reverberating reflections. These reflections occur between various reflectors, such as welds and discontinuities, including damage. The two methods are different but complementary. The first one involves the manual simulation of finite reverberating reflections, providing interpretable simulations that offer insights into how different reflections interact, especially in overlapping areas. The second method accounts for the scattering by all defects or discontinuities within the waveguide, resulting in a highly accurate simulation of the inspection since it accounts for infinite reflections. Although the complementary nature of accurate generative models versus interpretable generative models is well-known, it is less appreciated for physics-based modelling. This study clearly demonstrates the complementary nature of the two models for a validated field experiment from a damage-free rail containing welds and holes as discontinuities. The simulation results explore the synergy between these two methods, where one unravels reflection complexities, forming the foundation for interpretable back-and-forth reflections, while the other provides accurate simulations, accounting for all reflections in the waveguide. These insights can help to improve the reliability of guided wave-based monitoring systems.

Generalized Weak-form Free Element Method for Solving Mechanics Problems

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In this study, two generalization methods are proposed for extending the Weak-form Free Element Method (WFrEM) to solve heat conduction, solid and fluid mechanics problems by using general iso-parametric elements with and without internal nodes. The first generalization is performed based on the interface force/flux equilibrium of all elements around the collocation point as done in FEM and the second one is fulfilled by setting up a control volume within a free element as done in FVM. These generalizations can break through the restriction of FrEM on using elements having at least one internal node. Besides, the free element control volume method presented in this study can overcome the difficulty in FVM that high-order solution schemes cannot be easily formed. In the generalized WFrEM, also called the extended WFrEM, the meshes used in the standard FEM as well as the polygon/polyhedron elements can also be naturally used. Detailed formulations of the generalized WFrEM for solving heat and mechanics problems are given in the study and a number of numerical examples will be analyzed to verify the correctness and stability of the proposed method.

Numerical study of 3D metal cutting processes within the Material Point Method

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The Material Point Method (MPM) represents an alternative simulation technique as to e.g. the well-known Finite-Element-Method. In the MPM, bodies are discretized using material points while the equations of interest are solved on a computational background grid, see [1]. Within an MPM simulation, quantities of the material points are mapped onto the grid nodes of the computational background grid first, on which the degrees of freedom are solved, and then mapped back to the material points. This process enables the material points to move through an undeformed background grid in each time step, hence completely avoiding mesh distortion in the context of huge deformations as it occurs in e.g. FEM simulations. In this contribution, three-dimensional examples of vertical and horizontal metal cutting simulations are presented, taking into account the Johnson-Cook material law, see [2]. This plasticity law includes the influence of plastic strain rates as well as plastic heat that occurs during the cutting process. In addition, the grid-shift technique as introduced in [3] is employed which leads to a more physical material response.

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Mean zero artificial diffusion for stable finite element approximation of convection dominated problems

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In convection-diffusion problems, it is well-known that instabilities in finite element discretization may occur for convection-dominated problems. In this presentation, we develop a novel mean zero artificial diffusion method that circumvents such instabilities. Our methodology is efficient, accurate and does not smear the sharp gradients appearing in the solution. Allowing for equal-order finite element approximations for all fields of a coupled problem, the proposed framework proves to be computationally more robust when compared to a mixed-order finite element method. Using a general formulation applicable to chemomechanics or biomechanics, we provide proofs of the well posedness of the proposed methodology. Numerical examples are provided to illustrate the performance of the new approach.

Numerical Analysis of Blast Pressure using Blast Test Device

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Explosions, whether accidental or intentional, can lead to devastating consequences, causing 12% casualties, including severe injuries and fatalities, among 4765 patients analyzed from the Joint Theater Trauma Registry between 2003 and 2006. Notably, Primary Blast Injuries were observed in this study, with lung injuries being a significant contributor to blast-related mortality. To simulate and assess blast effects, a simplified rigid human torso surrogate, known as the Blast Test Device (BTD), was designed and tested. The BTD underwent exposure to complex blast waves in open-field conditions, generated by detonating 300 g of Plastic Explosive (PE4) at varying heights above a smooth, concrete surface. The experimental results were compared with both numerical simulations and existing data from literature. The computational analysis was conducted with the use of MSC Dytran. A half-symmetry 3D model. The comparison involved evaluating incident pressures, reflected pressures, and the positive phase duration of the blast wave. Overall, there were morphological similarities between the experimental and literature results. However, in three of the comparisons, there were time delays observed for initial peaks. Similarly, the numerical predictions exhibited good morphological agreement, but they also showed time delays for side-on pressures, as well as variations in initial peak pressures when compared to the experimental findings. This computationally constructed model exhibits the potential to serve as a valuable tool for facilitating future investigations on blast wave-structure interactions. Its successful validation enhances confidence in its capabilities to contribute to scientific research in this field.

Tumbling blocks: A study of non-spherical charge simulations and PEPT tracking validation for a tumbling mill geometry

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This project presents a comprehensive investigation into the simulation and tracking of non-spherical particles, including cubes and faceted polyhedral shapes, using Discrete Element Method (DEM) simulations and Positron Emission Particle Tracking (PEPT) techniques. The primary goal of this research is to validate the numerical model by comparing simulated particle behavior with experimental data obtained through PEPT. Non-spherical particles are prevalent in various industrial processes, including comminution, where they exhibit distinct behaviors compared to their spherical counterparts. Understanding and accurately modeling the dynamics of these particles are critical for optimizing process efficiency and equipment design. The validation of numerical models for non-spherical particles not only advances our fundamental understanding of granular materials but also has practical implications for comminution research. It enables more accurate predictions of particle behavior in tumbling mills and other comminution equipment, ultimately contributing to improved process design and energy efficiency. This project's findings offer a significant step forward in the field of granular simulations, bridging the gap between numerical modeling and experimental observation for non-spherical particles. Moreover, the validated models can be applied to a wide range of industrial processes beyond comminution, where non-spherical particles play a pivotal role.

Advances in Particle Finite Element Method for the Simulation of Phase Change Problems and Fluid-Structure Interactions

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Particle Finite Element Method (PFEM), see e.g. [1,2,3] for a state of the art, is a still rather young method that tries to combine the advantages of classical methods such as FEM and more recent methods known as particle methods (SPH…) The method is quite versatile and can be applied to both solid and fluids material behavior. It is a Lagrangian method that combines computations over one time step using FEM with a fast remeshing algorithm trying to avoid mesh distortions consequent to very large deformations such as the ones encountered for fluid flow with free surfaces. New developments will be presented here, such as the use of a level set function, instead of the traditional alpha-shape algorithm to determine the new boundaries of a body after remeshing, as well as the implementation of phase-change algorithm, including vaporization. The lecture will cover several applications including the simulation of the fluid behavior in a melt pool during LPBF (laser Powder Bed Fusion) where the initial powder is melted by the laser, and then solidifies again when the laser goes away. During this process, due to the high power density of the laser, some part of the material is not only melted but also vaporized. Other applications of the PFEM will illustrate fluid-structure interactions simulations including contact between different solid parts and plastic deformation of some components of the system.

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8. From Data and Models Towards Digital Twins

Digital Twins for Critical Infrastructure Protection

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System condition monitoring and risk prediction in the area of critical infrastructures (CRITIS) are of great importance for national security and state community. Especially for structures and technical facilities, virtual images that can be simulated and supported by data over their lifetime are particularly valuable. They improve the forecasting capability with regard to loads, maintenance requirements and incidents as well as for extreme and failure scenarios. In the long term, this can increase the resilience of the systems under consideration. Within the framework of the projects RISK.twin at the University of the Bundeswehr Munich as well as PhySimTwin at the German Aerospace Center (DLR), so-called "hybrid" digital twins for selected components of critical infrastructure are being developed on a broad scale, from basic scientific methodology (simulation, machine learning) to very specific application scenarios and objects (bridges, building construction, water, energy), and their usability for the responsible actors in critical decision-making is being investigated - both for civilian and military use. In this contribution, we give an overview of the current status of the two aforementioned projects as well as the already established collaboration network. Moreover, a methodological deep dive into physics-informed neural networks (PINNs) as one of the most promising techniques from the emerging field of scientific machine learning will be given alongside an outlook on their applicability in the context of critical infrastructure protection.

Digital Twins for Structural Health Monitoring on Offshore Wind Turbines

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To achieve the energy transition of many countries towards renewable energies, wind energy is very important. To meet the energy demand, not only more and larger wind turbines need to be built, also a reliable operation needs to be assured. This work will present the concept of a digital twin for structural health monitoring applications in wind energy. The focus is on transferring the state of the real turbine to the simulation model to realise a digital shadow first. To provide a simulation model, which can calculate the current state of the structure over its lifetime the structural model of the wind turbine needs to be updated. This is because of structural changes like damages and material fatique or changing boundary conditions like marine growth and scour. To do this, the modal parameters of both the simulation model and the real structure are compared. With model updating based on measurement data, real structural behaviour can be transferred back to the simulation model. Very important while doing this is to take into account the prevailing uncertainty in the measurements [1]. The measurement data is always attached with uncertainty because of the measurement error of the sensors, inaccuracies in the measurement chain and also due to the kind of processing the data. This uncertainty needs to be taken into account in the model updating to achieve a reliable result. In this work, a new approach to do this will be presented. The proposed method achieves similar output like state of the art methods, while reducing the computational time to a fraction. The method will be applied and compared on a laboratory steel beam with reversible damage mechanisms. [2] This allows comparing the results on a variety of different damage scenarios. The first four natural frequencies

related to pure vertical bending mode shapes are identified using the Bayesian operational model analysis (BAYOMA). BAYOMA is able to quantify the uncertainty in the natural frequencies.

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A new Mid-fidelity Aero-Hydro-Servo-Elastic Simulation Tool for Digital Twins of Large Offshore Wind Turbines

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The need to massively reduce carbon emissions is widely recognized. One major source for carbon-neutral energy production is wind energy, both onshore and offshore. Wind turbines have steadily grown in size in the past decades and are expected to continue to do so with diameters reaching up to 400 m and rated power of more than 20 MW. Such large wind turbines are large slender structures, which are much more prone to large deformations than current wind turbines. This means that nonlinear dynamic phenomena will become more dominant and the interactions between the different wind turbine components and the environment will have to be considered in detail. Current simulation tools for wind turbines rely on low-fidelity methods like Blade Element Momentum theory and linear beam models to achieve high computation efficiency, which is required during the design process. However, these intrinsically linear models might not be sufficient to deal with the nonlinear behavior of upcoming large wind turbines. Higher-fidelity methods, like RANS, are capable of capturing the physical behavior very well but their computational costs make their use unfeasible during the design process. As good trade-off between accuracy and efficiency, we suggest to use mid-fidelity methods, which consider the most important nonlinear phenomena intrinsically: The structure is modelled using a flexible multi-body system/finite elements approach with rigid bodies for hub and nacelle and geometrically exact beams for tower, blades and substructure, coupled by holonomic and non-holonomic constraints [1]. The air flow is modelled using the Unsteady Vortex Lattice Method, a well-established tool to compute the vortex dominated 3D flow of an ideal fluid around lifting as well as non-lifting surfaces. The nonlinear structural and aerodynamic equations are coupled based on the principle of virtual work. The hydrodynamic forces on the substructure are computed using the well-known Morison equation and for controllers an interface for Bladed-style controllers has been implemented. In combination with a monitoring concept and a model update strategy this model serves as core of the Digital Twin of a large offshore wind turbine. In this work, we summarize the theory on which our simulation tool is based as well as some exemplary comparisons between our tool and OpenFAST, a widely used current simulation tool, for the IEA-15MW-240-RWT reference wind turbine.

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Long-term Modelling of Asphalt Pavement Subjected to Traffic Load and Temperature Changes

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This study focuses on examining the response and observed deformations of asphalt pavement. These deformations arise from two main factors: first, short-term traffic loading (tire overrun), and second, temperature changes, which can be further categorized into two levels—day-night variations and seasonal temperature fluctuations. Numerous investigations have underscored the importance of precise numerical evaluation of the pavement structure for ensuring reliable and accurate long-term predictions. In this contribution, the structural longterm response of asphalt pavement subjected to periodic traffic loading and temperature changes is thermo-mechanically investigated. The pavement is modeled as elastoplastic solid at large strains within the framework of the Arbitrary Lagrangian Eulerian (ALE) formulation. To efficiently predict the structural response of the pavement due to repetitive tire overrun and thermal changes, time homogenization technique is employed. Time homogenization is used to address various time scales in the pavement's response, encompassing short-term loading (tire overrun), as well as day-night and seasonal temperature variations occurring over the span of several years.

Automatic Surface Adaption for As-is Pavement Modelling via Voxel-based Change Detection for Digital Twins of Pavements

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Accurate spatial-geometrical replication of pavement surfaces is vital for realistic simulations under various loading conditions and for predicting pavement distress within a digital twin. Currently, structure analysis using Finite Element Method (FEM) primarily focuses on pavement layer structures, while neglecting changing surface conditions. However, detailed knowledge about the pavement surface condition from the
real-world road environment is crucial for robust structural response simulations, as the actual loading condition is significantly influenced by the pavement surface [1]. Additionally, connecting real-world changes to simulation outcomes enhances the overall interpretability of processes related to structural aging [2]. In this contribution, we present an automated approach for as-is pavement surface modeling using voxel-based change detection derived from reality capturing data. The automated identification of pavement distress over time and its integration into existing digital models enables an essential step for the generation and maintenance of a digital twin. Furthermore, the resulting data can serve as a foundation for the adjustment of parameters in pavement-tire interaction models. Thereby, we establish a strong connection between structural health
monitoring and structural analysis, fostering a closer integration of both aspects within the framework of digital
twinning.

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Advection of Internal Variables in a Dynamic ALE Framework Enabling Fast and Accurate Predictions from a Digital Twin of the Pavement

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The Arbitrary LAGRANGIAN EULERIAN (ALE) formulation has been demonstrated as a convenient method to improve computational efficiency, particularly in the case of pavements subjected to moving wheel loads [1, 2]. This increase in computational efficiency is vital to a digital twin of the pavement, as it facilitates quick decision making. The extension of the dynamic ALE formulation of [2] to inelastic materials is needed, since the materials used in pavements exhibit inelastic behaviour. Such an extension would undoubtedly increase the accuracy of the predictions made by the digital twin of the pavement. The key challenge to be overcome in order to achieve this, is the advection of internal variables present in inelastic material models. This study aims to compare some of the methods already existing in literature to solve the advection of such internal variables, when inelastic material models are used in the dynamic ALE formulation.

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9. Reduction Methods

Deep Learning Model Compression for faster training and inference of surrogates for CFD boundary condition unceratiy quantification

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3D patient-specific computational models can provide valuable insights into the heamodynamic and biomechanical conditions of a patient's cardiovascular system for both intervention and post-operative care planning. However, their translation into real clinical settings is limited and in resource constrained settings their design requires greater consideration. Our approach in aiding the translation of patient-specific modelling pipelines into the clinical setting is by using doppler echocardiography for velocity data acquisition as opposed to phase contrast magnetic resonance imaging (PC-MRI) as is commonly used within the literature to prescribe inlet and outlet boundary conditions. Inlet and outlet boundary conditions have a strong influence on the accuracy of the numerical used and has been closely studied within the literature. Furthermore, the use of doppler echocardiography introduces uncertainty due to the operator (as measurements strongly dependent on operator skill level), the nature of the device (time discontinuities between measurements) and patients physiological state (variations in heart rate or volumetric flow rate). These uncertainties must be considered when prescribing inlet and outlet boundary conditions as well as their effects on the flow metric calculated using the computational model. However, uncertainty quantification methods such as the Monte Carlo (MC) method and the Generalized Polynomial Chaos Expansion (gPCE) method require several evaluations and running 3D CFD simulations is computationally expensive especially in limited compute environments. Therefore, it is preferrable to use reduced order/surrogate methods that are computationally cheaper but accurate. Deep Learning based surrogate models have been introduced to calculate patient haemodynamics within the literature. However, these models have can take long to train and the main benefits of a speed up is at inference. Thus, challenging the benefit of using them as surrogates as opposed to traditional numerical approaches. Recent strides in deep learning model compression has seen the reduction in training and inference times in the domains of natural language processing and computer visons. The set of compression methods used fall into the following categories pruning, quantization, distillation and low rank factorization. Thus, in our work we explore the application of these methods to create surrogates for boundary condition uncertainty quantification for a patient specific CFD model.

10. Structural Mechanics, Stability and Dynamics

Fluid-Structure Interaction Analysis of Rotating Shaft with Stator Contact in Incompressible Fluid

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During rotor-stator contact, fluid interaction between the rotating machinery plays a crucial role in concealing the maximum stress limit, which may gradually damage the rotating machinery. When an oscillating shaft comes into contact with a fixed stator, it develops fluctuating stresses at the point of impact as the system's stiffness changes according to the contact state. Integrating Fluid-Structure Interaction (FSI) analysis into dysfunctional rotating systems is crucial due to its intrinsic attributes, which are associated with examining flexible structures capable of undergoing deformation in response to fluid motion and thermal effects. This paper examines the investigation of the imbalance and rotor-stator contact on a rotating shaft, which is modelled as an elastic vertical rotor operating in an incompressible fluid. The first step involves formulating the implicit representation of the rotating system, which includes the rotor-stator contacts and the hydrodynamic resistance for the coupled system. This formulation is established by using the energy principle and the Navier-Stokes equations. Furthermore, the implicit strategy of the rotor-stator fluid interaction interface condition is included in the solution methodology using a monolithic approach that combines the algorithm and formulates a single system of equations. The major reason for frequency fluctuation may be attributed to time-varying stiffness resulting from friction, as shown by the historical records of vibration displacement, whirling orbit patterns of the centre shaft, and the amplitude-frequency curve. Additionally, it has been shown that the temperature impact on the rotor's movement leads to an augmentation in the magnitudes of the flow perturbations, resulting in a decrease in its oscillation.

A hierarchical Snap-through model for Mimosa Pudica leaf folding kinematic

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Mimosa Pudica (MP) displays a hierarchical leaf-folding response to external disturbances [1]. This rapid movement, as seen in other plant species [2], relies on the mechanical adjustment of tissue pressure through osmotic regulation in specific structures, known as pulvinulae in the case of MP. Depending on the stimulus's intensity and location, the resulting motion can range from the movement of a pair of leaves to the collapse of the entire branch. Due to this progressive on-off behavior, the folding system has been modeled as the linear buckling of a concentrated linear elasticity system. This is achieved through rotational springs and by considering a straightforward time function for electrochemical signaling. By tracing each stimulus back to a bending stimulus at the pulvini level, a new perspective within the sensing-acting framework is proposed: shifting from an 'avoid-touch' interpretation to a 'bending sensitivity' approach.

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Materiality and criticality for Mimosa Pudica structural intelligence

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Mimosa Pudica (MP) has continually captivated scientists across various fields and disciplines. Alongside specialized insights from botany, biomechanics, and chemistry, recent research has shed light on the adaptive framework governing the leaf's movements [1]. This framework appears to have a primordial learning mechanism, distinguishing between environmental and loading characteristics. Employing a structural model of the pulvinus (as discussed in a companion paper), we utilized a critical modal likelihood to identify and interpret the adaptive behavior. The hierarchical stiffness model has been fine-tuned to match the overall stiffness through load-Euler modes [2]. We designed a sophisticated sensing-actuating apparatus to intricately relate to the structural morphology. Lastly, we harnessed the tuned buckling loads to train a neural network for modeling the learning process pertaining to the equilibrium, MP material intelligence, and morphological features.

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Modelling and Experimental Study of Eccentricity in Two-Stage Spur Gear Systems

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This study aims to examine the dynamic characteristics of spur gears with eccentricity faults by accurately establishing a mesh stiffness model. A two-stage spur gear model with ten degrees of freedom is employed, considering both gear eccentricity and dynamic transmission error. The Lagrange equation is utilized to derive the differential vibration equations for spur gear systems, incorporating the coupling between lateral and torsional vibrations to account for gear dynamics. The focus of this research is to extract and analyze the characteristics of two-stage spur gears, such as frequency variation and gear eccentricity during passage through critical speeds. Numerical simulation analyses are conducted using a combination of the short-term Fourier transform (STFT) and the RPM-frequency mapping technique under various operating scenarios for the system. The theoretical findings on dynamic behavior and eccentricity error detection in gear transmission are experimentally validated on two-stage spur gears. Compared to conventional time domain and power spectrum FFT, the proposed technique reduced signal noise and captured the one-period dynamics of the vibration signal. The study successfully identified the eccentricity error of the gear and its correlation with transmission error, providing valuable insights for backlash correction and control. The theoretical analysis aligned with experimental results, affirming the effectiveness of the STFT-based frequency-RPM transmission error detection approach.

Progressive Analysis of a Nonlinear Electromechanical System Sensitive to Initial Conditions by the Poincare Method

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This article describes the dynamics of a five-degree-of-freedom manipulator. A nonlinear dynamic model of the manipulator's arm is developed using Lagrangian formalism, which accounts for the variation between the system's kinetic, potential, and Rayleigh energy. The proposed DC gear motor coupled with a robotic hand model is then implemented in MATLAB considering the perturbation terms in joint arm angles and tested under real operating conditions for verification and validation. To optimize the model's performance, the parameters are refined using the bifurcation algorithm for nonlinear perturbation and motor parameters. The Poincare series-based controller also exhibited generally better performance, as shown by the lower average and maximum deviations from the unstable steady state. The results show that adjusting the model's parameters leads to improvements, highlighting the significant influence of these input data values on the validation results. Additionally, during the parameter estimation process, a connection between the parameters becomes apparent, suggesting that these values not only impact the validation results but also interact with each other. Overall, this study provides an effective theoretical guide for the vibration reduction of flexible human hands.

Investigating Robustness to Instability Against Imperfections of a Gridshell Roof in Dakar

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In structural engineering and architecture, gridshell roofs are widely used because they cover vast areas without the need for pillars or interrupting walls. These constructions consist of slender structural elements combined with glass panelling to allow natural daylight. Gridshells have intrinsic structural robustness due to their distinct shape. In any case, the structural geometry and slenderness of the main structural components make them vulnerable to instability phenomena [1]. In this work, the case study of the Dakar mosque gridshell roof is investigated with respect to robustness to global buckling. Two form-finding methodologies are employed to define the roof geometry. The Multibody Rope Approach (MRA) [2] and the improved Multibody Rope Approach (i-MRA) are form-finding methods specifically developed for free-form gridshell structures. The two structural shapes are studied with non-linear analyses to assess the impact of structural element slenderness and material non-linearity. Furthermore, geometric deviations are introduced in the numerical model to study the robustness of the structure with respect to imperfections. Different patterns of imperfections are defined by combining and rescaling the linear buckling eigenshapes for both structures [3]. Incremental load geometrical non-linear analyses (GNIAs) and incremental load geometrical and material non-linear analyses (GMNIAs) are employed to compute the equilibrium paths. The elastoplastic constitutive law is introduced in the GMNIAs to model the behaviour of structural steel. Finally, a deep investigation of the postbuckling behaviour of the structure is provided.

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Dynamic Responses of Dielectric Elastomer Structures

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We summarize in this report the recent advances in our study of dielectric elastomer (DE) structures in general and plates/shells in particular. DEs, as a typical type of smart materials, are usually very soft, and deform significantly when subjected to electric and mechanical stimuli. Thus, we need to employ the general nonlinear theory of electroelasticity to take account of both the geometric and material nonlinearities. A typical and most recent version of the theory was suggested by Dorfmann and Ogden. Also, we need to employ the incremental linear theory for elastic waves superimposed on large deformation. The static large deformation induced by a pre-applied mechanical force or electric stimulus changes the geometry as well as the instantaneous material properties of the structure, and can be an efficient approach to tuning the dynamic behaviors of soft DE plates and shells. We have researched the vibrations and wave propagation characteristics in typical DE structures, including circular and rectangular plates, cylindrical shells and spherical shells. For these structures with relatively simple geometries, we have been able to derive exact solutions for particular types of pre-deformations. Also, we have taken account of structural periodicity to consider waves in DE phononic crystal structures.

Deformation Behaviour, Limitations in Design, Applications, and Additive Manufacturing of Hierarchical Honeycombs

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Hierarchical honeycomb structures are particularly advantageous in the aerospace industry as a result of their ability to overcome challenges related to bend-dominated behaviour. These structures are ideal for aeronautical applications because of their capacity to integrate lightweight design, good mechanical properties, and efficient load distribution. However, the efficacy under applied loads is influenced by the type of polygon cell introduced at the vertices. The current literature has gaps in knowledge with reference to the highest order of hierarchy that can practically be achieved for hierarchical honeycomb structures with different cell shapes at the vertices.

This paper presents an overview of hierarchical honeycomb structures with triangular, hexagonal, and circular cells substituted at the vertices, with the aim of examining their mechanical properties and how efficiently they can be designed. In the first section, existing, and relevant analytical models in the literature, on the mechanical properties of hierarchical honeycomb structures are identified and discussed. These include Vogel's model for hierarchical honeycombs, the Gibson and Ashby models, and the Castigliano methods, which are typically employed for analytical modelling of the behaviour of hierarchical honeycomb structures. Though these analytical models are built using the relationships that exist between connecting vertices, they fail to account for the deformation behaviour at these points. This is followed by the second section, focusing on determination of the constraints in the order of hierarchy for these structures, particularly the geometric parameters.

The highest order of hierarchy, presently feasible, is observed for a second-order hierarchical honeycomb structure with hexagonal cells at the vertices. Furthermore, the hierarchical structuring of honeycomb structures is limited by geometrical parameters, including the edge length ratio, cell angles, and the ratio of thickness to edge length. In the third section, a review of relevant applications for hierarchically built honeycomb parts in the aerospace industry is presented. The aerospace industry typically builds lightweight structural parts, capable of absorbing high strain energies through the use of hierarchical honeycomb designs. It is observed in this paper that the hierarchical honeycomb

structure comprised of triangular cell substructures at the vertices has the greatest capacity for absorption of energy of the three first-order hierarchical structures studied here. Finally, the efficacy, as well as challenges of using additive manufacturing for building hierarchical honeycomb structures are discussed, noting that additive manufacturing is challenged by the geometric intricacy and complexity of hierarchical honeycomb designs, as well as the minimum resolution that can be printed, a constraint that increases with increasing order of hierarchy.

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11. Control Theory and Optimization

Implicit Peer Triplets in Gradient-Based Solution Algorithms for ODE Constrained Optimal Control

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Recently, we have developed and analysed implicit two-step Peer triplets for nonlinear ODE constrained optimal control problems [1,2]. We combine some standard Peer methods for inner grid points with carefully designed starting and end methods to achieve order four for the state variables and order three for the adjoint variables in a first-discretize-then-optimize approach. The notion triplets emphasizes that these three different Peer methods have to satisfy additional matching conditions. These methods do not suffer from order reduction – a phenomenon that is usually observed for one-step methods as e.g. symplectic Runge-Kutta methods. Peer methods compute several stages of equal (global) order per time step. They exhibit good stability properties, making them very attractive for stiff problems [3]. In this talk, we will present novel implicit two-step Peer triplets, which can be applied together with a projected gradient method [4]. The key observation is that such methods have to satisfy further positivity and consistency conditions. We will show results for a stiff method-of-lines boundary control problem for the heat equation in a comparative study and for continuous optimization of large-scale gas networks as described in [5].

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12. Coupled and Contact Problems

Soil penetration by passive and active probes: from geomechanics to mechanobiology

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Some classical topics such as the resistance offered by granular media to penetration of probes and the prediction of the bearing capacity of piles are receiving renewed attention from a different perspective, namely, bio-inspired robotics and biomedical engineering. Steerable needles and smart flexible catheters are being conceived following the inspiration provided by earthworms and roots moving in the soil [1]. Here, the probe is active, it is subject to muscular contraction or growth, and it moves inside biological tissues which behave as a passive medium over short time scales. Often, these are modelled as granular materials, and classical approaches resolving the complex inelastic response of soils need to be adapted to the case where the surrounding medium is a living tissue. At the same time, modeling phenomena such as pile heaving due to soil thawing, induced by global warming, require modeling the soil as an active medium inside which a phase transformation takes place [2]. This phase transformation powers the motion of the pile. The design of remediation measures can take advantage of tools developed for the study of the motion of natural and robotic seeds designed to penetrate spontaneously in the soil, by exploiting only environmental stimuli such as temperature, light, and humidity variations [3]. In this talk, we will review recent efforts from our groups to tackle challenges and opportunities offered to computational mechanics by the need to resolve the motion of active or passive probes inside active or passive granular media. Our results show that the study of the interactions between living organisms (earthworms, growing plant roots) can inspire new and effective solutions to problems in the fields of medical robotics and geotechnical engineering. Partial support for this research has been provided by the European Union through Horizon 2020 project I-Seed (https://iseedproject.eu/) and Horizon Europe project MapWorms (https://www.mapworms.eu).

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Unsteady Aerodynamics and Aeroelastic Phenomena of a Launch Vehicle with hammerhead nose

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Buffet is a turbulent, unsteady aerodynamic phenomenon characterized by fluctuation pressure resulting from flow induced turbulence, flow separation, wake effects, and shock oscillations. These fluctuating pressures can produce significant loads on a launch vehicle and spacecraft during ascent to orbit. The mission of a launch vehicle might be failed if the beffecting phenomenon happens in flight. Hence, to secure the design method predicting and preventing the buffet instability of a launch vehicle in flight is very important for its development. In this study, the unsteady aerodynamic forces of a launch vehicle with hammerhead nose are calculated by using CFD code. Also, The CFD-CAE coupled analysis method is developed and is used to calculate the aeroelastic response of a launch vehicle with hammerhead nose and predict the buffeting of the launch vehicle in flight. Self-sustained oscillation of a launch vehicle causes by aeroelastic coupling is investigated and the results are compared with those from the CFD-CAE coupled analysis.

Dual-phase lagging thermoelastic damping in plate resonator based on higher-order shear deformation plate theories

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Thermoelastic damping (TED) in high frequency resonator shifts its natural frequencies and attenuates the vibration amplitude. The amount of damping depends upon the temperature change in the device produced by the thermoelastic coupling vibration of the micro- or nano- structures. So, to accurately evaluate the TED is crucially important for the design of high-quality resonators. From the review of the previous investigation on the TED in micro/nano plates, nearly all the of mathematical models for the thermoelastic vibration of the plates were formulated based on the Kirchhoff plate theory where the effects of transverse shear deformation and the rotational inertia forces on the vibration response was ignored. Here, we consider a micro/nano rectangular plate with the four edges are simply supported. The governing equations for the vibration are established based on the Levinson higher-order shear deformation plate theory where the transverse shear deformation is estimated by both the sinusoidal and the hyperbolic shear stress shape functions. Two-way coupled heat conduction equation is derived based on the dual-phase-lag generalized heat conduction theory considering the effect of the time relaxation. Inverse quality factor representing the TED in the plate is extracted by using the complex frequency approach. Numerical results are presented to show the variation of the TED versus the physical and geometrical parameters of the plate resonator. By comparing the values of TED based on the Levinson plate theory with those based on the Kirchhoff plate theory, the level of effects of the shear deformation on the TED is analyzed in detail. The numerical results show that for the moderate thick and thick plate resonators the values of TED evaluated by the classical plate theory are obviously great than that by shear deformable plate theory. It is because that the classical plate theory ignores the transvers shear deformation and over estimates the rigidity of the structure. In addition, we analyzed the effects of the lagging times on the TED in the plate resonator. The numerical results illustrate that for the micro-sized plates the effect of the relaxation times on the TED can be ignored, however, for the nano-sized resonator the effect is obvious and it needs to be considered.

A fully coupling model for lithium diffusion and finite elastoplastic bending of bilayer electrodes in lithium-ion batteries

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A fully coupling model for diffusion induced finite elastoplastic bending of bilayer electrodes in lithium-ion batteries is proposed. The effect of mechanical stress on lithium diffusion is accounted for by the mechanical part of chemical potential derived from Gibbs free energy along with use of logarithmic stress and strain. The governing equations along with initial and boundary conditions are derived and solved by the finite difference method along with Newton-Raphson iterative scheme. Eight dimensionless parameters, which govern the stress-assisted diffusion and the diffusion induced elastoplastic bending, are identified. It is found that the finite plasticity starting from the interface of bilayer increases the chemical potential gradient and thereby facilitates lithium diffusion. The full plastic flow makes the abnormal lithium concentration distribution possible that the concentration at the lithium inlet is lower than the concentration at the interface (downstream). The increase in thickness of active layer during charging is much larger than the eigen-stretch due to lithiation, and this excess thickening is found to be caused by the lithiation induced plastic yield.

13. Interface Mechanics: Modelling and Computation

Adhesion and Friction: a Survey and a Unified Formulation

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It is first proposed to briefly review Cohesive Zone Models (CZM) and some more general models combining unilateral contact, adhesion and friction. Adhesion is taken to be a form of interface damage. The most widely used cohesive zone models are first discussed. The RCCM (Raous-Cangémi-Cocou-Monnerie) model is widely presented. It couples unilateral contact, friction and adhesion and considers the effects of viscosity. It is based on convenient choices for the free energy and the dissipation potential. The variational formulation set as a variational inequality and some associated solvers are briefly recalled in the context of non-smooth mechanics. In a second part, an axiomatics for adhesive interfaces, based on the unified model proposed by Del Piero and Raous is presented. This unified approach is based on:

- general laws, typically, energy conservation and dissipation principles, i.e., mechanical versions of the first two laws of thermodynamics,
- a set of state variables, i.e., a set of independent variables which entirely determine the response to all possible deformation processes,
- a set of elastic and dissipation potentials, which are functions of state in terms of which the general laws take specific forms,
- a set of constitutive assumptions.

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Numerical influence analyze of simulation of different design working conditions on deformation behavior of bridge bearing

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Polymers and composites based on them are used in a wide range of industrial applications. In particular, these materials are used as protective coverings, sliding layers, etc. There are many studies of polymers directed at revealing their deformation behavior under different operating conditions. However, few studies are conducted with simultaneous consideration of a large number of emerging factors such as: geometric characteristics of the product, choice of material behavior model, rheology, thermo-viscoplastic behavior, cyclic loads, etc. Therefore, studies on the deformation behavior of polymers under real working conditions are relevant. In our work, we are concerned with modeling the performance of the structure under realistic conditions. For the initial stage, numerical studies have been performed in ANSYS Mechanical APDL application software package. The article considered a numerical model of bridge bearing manufactured by "AlfaTech" of Perm Russia. This structure consists of two steel plates with a spherical indenter and cutout, as well as a sliding layer between them. PTFE is considered as the sliding layer. The paper analyzed the influence of a large set of geometrical characteristics, such as: the sliding layer thickness, the penetration depth into the lower steel plate, the sliding layer location, the angle of the layer inclination, the nature of the contact interaction between the surfaces [1]. Also the influence of mathematical model behavior of polymers such as: elastic body, elastic-plastic, viscoelastic was considered [2]. The friction coefficient influence between the contact surfaces has been investigated. All the above parameters, in one way or another, affect the deformation behavior and contact parameters of both the sliding layer and the bearing. The next research stage is modeling of bearing operation under the cyclic loads influence, seismic impact, taking into account the temperature influence, as well as the polymers rheology.

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Numerical identification of constitutive relations of viscoelastic and viscoplastic of lubricants behavior

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Lubricants are widely used to increase the service life of polymer protective antifriction layers and reduce their frictional wear in the bridges bearings [1]. The lubricant in the structure is in a state of hydrostatic compression, which makes it possible to behavior model of materials using Maxwellian-type equations. Building models of the lubricant dynamic behavior is one of the current problems [2]: viscoelasticity, viscoplasticity, etc. A series of experiments to determine the thermomechanical and rheological properties of lubricants was carried out in the work. A numerical algorithm for identifying constitutive relations has been constructed. The 4 lubricants were considered as objects of study: CIATIM-221, CIATIM-221F, TOMFLON SBS 240 FM and TOMFLON SK 170 FH. The experiments were performed over a wide range of temperatures [- 40;+80] °C and strain rates [0.01; 100] Hz. The constitutive relations of the Prony series and the Anand model are chosen to describe the materials thermomechanics using the Williams-Landel-Ferry temperature-time analogy. The numerical algorithm also includes the Nelder-Mead optimization method, ensuring an error of no more than 5%. The identification procedure is based on the Python programming language and numerical simulation of a pure shear experiment in the ANSYS Mechanical APDL application software package. It has been established that the presented approaches make it possible to quite effectively describe the behavior of lubricants at high strain rates. A comparative analysis of the deformation behavior of lubricants on model and test problems has been performed.

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14. Damage, Fracture and Failure

Investigating the Fatigue Life of High Temperature Annealed DMLS TI6AL4V(ELI) at Elevated Temperature

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Though failure of engineering materials has been studied extensively, complete prevention of failure is never guaranteed. The present study aims to investigate the effect of elevated temperatures on the fatigue life of Ti6Al4V(ELI). A DMLS EOSINT M290 machine was used to manufacture test specimens. The specimens were further machined to comply with ASTM E466 standard for fatigue testing. Stress relief and high temperature annealing heat treatments were applied on specimens to remove residual stresses arising from the additive manufacturing process and to transform the as-built microstructure, respectively. Thereafter, fatigue tension-tension tests were carried out on the specimens at the different temperatures of 20 °C, 175 °C, 325 °C, and 475 °C. These test temperatures were selected to determine the trend in fatigue life of the alloy as the test temperature is increased from 20 °C to 175 °C, 325 °C, and 475 °C. The Ti6Al4V(ELI) alloy is limited in its applications up to a temperature of 400 °C, as temperatures above 400 °C can affect its microstructures and ultimately its fatigue life. The temperature of 475 °C was selected to confirm this limitation for the application of the alloy. The test was carried out at different maximum stresses of 80, 70, 60, 50, 40, and 30 % of the yield strength and a constant stress ratio of 0.1, till failure or attainment of 5,000,000 test cycles. The results obtained showed that the fatigue life of Ti6Al4V(ELI) was dependent on the test temperature.

Computational Mechanics for Superstrong Materials

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Among the strongest nano-materials one is recognized as iconic: carbon nanotubes, with theoretical strength estimated [1] and recently measured to be up to 70-90 GPa. Over decades, however, to harness such strength in any form of macroscopic material like a fiber or a rope, cable, remained a challenge. We will discuss multiscale computational models developed and employed over recent decade which allow one to understand the causes of the apparent macroscopic assembly “weakness” (often below 1 GPa) and how both strength and toughness can be improved through interface engineering, currently reaching in laboratories ~10 GPa, in par with best commercially available carbon fibers. We will also discuss computational models elucidating the nature of fatigue [2] in carbon nanotubes fibers as a collective phenomenon, while also demonstrating that intrinsically each nanotube is essentially indefatigable, per se. Prospects for further strength increase through chemical functionalization, or an alternative of boron-nitrogen (BNNT) constituents [3] will also be discussed, and how this progress can be guided by multi-physics computational mechanics models, from quantum chemistry of covalent bonding to the lateral load transfer and overall mechanical strength.

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A multiscale phase-field fracture approach for rubber-like materials accounting for anisotropic network responses

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The study of elastomers has recently gained substantial attention due to their expanding range of applications. These materials exhibit remarkable properties, primarily stemming from their intricate polymer chain network, which, in turn, increases the complexity of precisely modeling their behavior. Especially for modeling their fracture behavior, accurately accounting for the deformations of the polymer chains is vital for predicting the rupture in highly stretched chains [1,2]. Despite the importance, many robust multiscale continuum frameworks for modeling elastomer fracture tend to simplify network deformations by assuming uniform behavior among chains in all directions. Recognizing this limitation, our study proposes a multiscale fracture model that accounts for the anisotropic nature of elastomer network responses. At the microscale, chain damage is assumed to be driven by both its entropy and the internal energy due to molecular bond distortions. To bridge the stretching in the chains to the macroscale deformation, we employ the maximal advance path constraint network model [3,4], inherently accommodating anisotropic network responses. To drive macroscale fracture based on damages in these chains, we utilize micromorphic regularization. Finally, a thermodynamically consistent phase-field continuum formulation is proposed. Additionally, to enhance our understanding of the fracturing process, we conduct uniaxial tensile experiments on a square film with a hole and then compare our simulation predictions with the experimental observations. Furthermore, we visualize the evolution of stretch and damage values in polymer chains oriented along different directions to assess the model's predictive capacity. The results are also compared with another existing model to evaluate the utility of our approach in accurately simulating the fracture behavior of rubber-like materials.

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Soft Fracture of Dielectric Elastomers: Experiments and Modeling

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The increasing interest in smart materials owes to their capacities to adjust their mechanical properties and perform morphology changes under external non-mechanical stimuli. Among others, smart structures can respond to magnetic, light, chemical, acoustic, and electric stimuli. Soft dielectric elastomers undergo large alterations in their material characteristics when exposed to electric stimuli. The response is initiated by Coulomb forces within the material, which translate the electric field into a mechanical reaction. To achieve this, flexible electrodes are attached directly onto the elastomer. Applications involving large deformations can lead to the emergence and spread of cracks. In this context, the electro-mechanical actuation on dielectric elastomers can impact their fracture performance. In the work that we present here, we delve into the fracture behavior of extremely soft elastomers with intial pre-cuts. To that end, we perform tensile tests with a custom-made testing setup that allows to couple the mechanical deformation with the application of electrical stimulation. Furthermore, we investigate the effects of embedding piezoelectric BaTiO3 particles within the elastomer. Concurrently with these experiments, we employ a bespoke fracture phase-field model to explore the stress triaxiality state in the vicinity of the crack tip driven by the lateral contraction produced by the Coulomb forces. The model integrates the electro-mechanical coupled problem with damage evolution. In addition, we calculate the nodal configuration forces and compare virtual experiments without and with electric actuation. The comprehensive analysis indicates that the electric stimulation leads to beneficial blunting of the crack tip that decreases the stress concentration, enhancing the work to fracture by up to a 125% and delaying crack propagation. Additionally, the incorporation of fillers amplifies the effect beyond the limits observed in unfilled elastomers. This research opens new routes to potential applications of soft dielectric elastomers in advanced scenarios where enhanced fracture properties are required, or more broadly, a tailored fracture behavior.

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A Coupled Implicit Material Point – Finite Element Method for Fracture Simulation by the Eigenerosion Approach

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While using the Finite Element Method (FEM) in the fracture simulation problems, the mesh distortion problem is often limit the simulation from addressing the complete response of structural elements. To overcome this issue the Material Point Method (MPM) is a good candidate as, due to the mesh resetting characteristic, the problem of mesh distortion is avoided. This study is focused on the numerical simulation of fracture via the combination of the FEM and the MPM, utilizing the beneficial features of both approaches, whilst attempting to mitigate their limitations. These two methods are combined within a monolithic implicit solution algorithm where both the finite element problem and the degrees of freedom of the material point method background grid are solved simultaneously. The unknowns on the two grids/meshes are coupled via a penalty approach that limits the separation between the active elements of the MPM and the adjacent finite elements, such that artificial gaps/overlaps do not appear within the physical body being analyzed. This framework is used as the basis of fracture simulations via the automatic conversion of finite elements into material points based on an eigenerosion criteria. The eigenerosion technique is used to degrade the stiffness of fractured material and allow large deformation crack opening, with branching and merging of fractures if appropriate. The key benefit of converting finite elements to material points after being eroded is that it avoids the finite element mesh distortion that can occur when modeling large deformation fracture mechanics.

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15. Data Science and Machine Learning

Latent Space Perspicacity and Interpretation Enhancement (LS-PIE) Framework

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Linear latent variable models such as principal component analysis (PCA), independent component analysis (ICA), canonical correlation analysis (CCA), and factor analysis (FA) identify latent directions (or loadings) either ordered or unordered. The data is then projected onto the latent directions to obtain their projected representations (or scores). For example, PCA solvers usually rank the principal directions by explaining the most to least variance, while ICA solvers usually return independent directions unordered and often with single sources spread across multiple directions as multiple sub-sources, which is of severe detriment to their usability and interpretability. This paper proposes an analysis approach to enhance latent space representations for improving the interpretability of linear latent spaces. This frame-work automates the clustering and ranking of latent vectors to enhance the latent information per latent vector as well as the interpretation of latent vectors. Several methods are incorporated including latent ranking (LR), latent scaling (LS), latent clustering (LC), and latent condensing (LCON). These approaches are wrapped into a framework implemented in Python. For a specified linear latent variable model, LR ranks latent directions according to a specified metric, LS scales latent directions according to a specified metric, LC automatically clusters latent directions into a specified number of clusters, while, LCON automatically determines the an appropriate number of clusters into which to condense the latent directions for a given metric. As the data of most engineering problems falls broadly into two domains: single channel and multichannel data additional analysis have been included for these sources using data preprocessing strategies such as Hankelization to seamlessly expand the applicability of linear latent variable models (LLVMs) to a wider variety of data. The effectiveness of LR, LS, and LCON are showcased on both crafted foundational problems as well as on practical vibrational problems to showcase the usefulness as well as the importance and feasibility of improved latent representations.

Causal Discovery and Counterfactual Recommendations for Personalized Student Learning

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Predicting student performance and identifying students at risk of failing is indeed important. However, we believe that a more important problem is identifying the causes of being at-risk. If we do not know what is causing a student to fail, how can we provide personalized recommendations to advise students how to pass? In this study we introduce the need to move beyond predictive models to also identify causal relationships and structure in the data. Causal discovery methods are proposed as the way to achieve this [1]. Causal discovery refers to a host of statistical (and other) methods that aim to identify the true underlying causal structure in the data. Once we have the causal structure, we are then in a position to carry out causal inference and counterfactual analysis. This study's main contributions include using causal discovery to identify causal predictors of student performance and applying counterfactual analysis to provide personalized recommendations. We describe the application of a causal discovery method called PC-algorithm to real-life engineering mechanics student data. We show how this method can uncover potential causal structures which are plotted via a directed acyclic graph (DAG).

The results show that prior mathematics grades are causal to the performance in engineering mechanics. We then use causal inference methods based on the causal graph to estimate causal effects and generate counterfactual scenarios, according to the method described by Pearl [2]. We show how counterfactual analysis can be applied by randomly selecting a failing student in order to provide individual personal recommendations to change their failure prediction to passing. This method promises much for any field where we require the underlying causal structure (i.e. the data generating process) and for applications that require personalized recommendations such as education or medicine. Limitations of this method include the reliance on domain expertise for accurate causal discovery, and the necessity of larger sample sizes for reliable results. The potential for incorrect causal structure estimations is also acknowledged. A major challenge remains, which is the real-time implementation and validation of counterfactual recommendations. In conclusion, we demonstrates the value of causal discovery for understanding student performance and providing personalized recommendations.

Non-linear Regression Analysis for Prediction of Mandible Cephalometric Measurements

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Accurate assessment and prediction of mandible shape are fundamental prerequisites for successful orthognathic surgery. Past evaluations of three-dimensional cephalometric norms have shown moderate to strong linear relationships between upper facial dimensions, such as facial height and width with jaw measurements [1,2]. Notably, only poor relationships were found between measurements concerning solely the maxilla or cranium and those involving the mandible [2]. However, it is possible that these relationships could be better described through a non-linear approach. In this paper, a comparative analysis was conducted between non-linear models and representative multiple linear regression models. The non-linear models include a multilayer perceptron network, a mixture density network, and an ensemble random forest model. The models were fitted on a measurement dataset derived from 156 publicly available CT scans. An exclusion protocol was used to ensure consistent scan parameters and the absence of visible bone pathology or significant scan artefacts. Subsequently, the scans underwent segmentation to isolate the cranium and mandible while removing scattering. The resultant meshes were then annotated with typical landmarks from which the cephalometric measurements were defined. Non-linear models are expected to outperform the traditional linear model in predicting measurements in the presence of non-linear relationships between upper-facial and mandible measurements. This result could assist clinicians in planning orthognathic surgery and inform future research when considering the relationship between the cranium and mandible.

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Estimation of coal GCV via live plant data

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The amount of heat released upon complete coal combustion is known as the gross calorific value (GCV), also referred to as the higher heating value (HHV) of coal. The GCV of coal is a parameter that must be readily available because it is one of the crucial elements that can be used to determine boiler heat balance, thermal efficiency, and boiler output [1]. Differential scanning calorimetry (DSC), linear and non-linear regression, and artificial intelligence (AI) techniques are now utilized to estimate the GCV of coal. These techniques need the proximate and ultimate analyses of coal as input parameters. The difficulty with these procedures is that they include complex equipment that requires specialized operation, making it a time-consuming task to estimate the GCV of coal. This study focuses on using live plant data as input parameters to estimate the GCV of coal. A distributed control system (DCS) used in power plants records plant process characteristics every second. DCS data will be extracted from the DCS and applied on a non-linear regression analysis will be conducted to analyze the correlation between the GCV of coal and live plant data. The method will help with the ongoing monitoring of coal's GCV.

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Overall arrangement for oppStudio: A novel computation software for multi-omics data analysis

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Bioinformatics interprets the mechanisms of entire life cycle through the analysis, integration, and interpretation of massive biomedical data, which involves a wide range of fields such as sequencing data analysis, single cell data analysis, spatial transcriptome data analysis, protein interaction networks, signal pathway analysis and simulation, metabolic flow analysis, RNA network analysis, three-dimensional protein structure prediction, drug virtual screening, microarray analysis, mass spectrometry data analysis, and medical imaging data analysis. We have developed OPP (Omics Pilot Platform), a series of software that focuses on omics data analysis. Here we presented three mature modules in OPP, including oppOntology for enrichment analysis, opplncRNA for lncRNA pathway search and oppHeatmap for personalized heatmap construction. 1) oppOntology, an enrichment calculation application has been developed to calculate enrichment analysis for the target gene list by MATLAB, which supports online mapping of KEGG pathway diagrams in a batch way. oppOntology was designed not only for generic functional databases, but also for self-defined functional category databases. Customized GO terms slim was also supported by oppOntology. Meanwhile, oppOntology supports simultaneous calculation of multiple samples with manifold enrichment scores. 2) opplncRNA, a novel rapid tool for investigating lncRNA-miRNA-mRNA pathways for human species. It is useful to analyze the regulatory interaction networks of lncRNA with a friendly Graphical User Interface (GUI). Three lncRNA databases about lncRNA-miRNA interactions that have been integrated into opplncRNA, as well as seven miRNA databases about miRNA-mRNA interactions. opplncRNA can read expression data from any profile, such as microarray or RNA seq. Besides, the relationships between lncRNA-miRNA and miRNA-mRNA can be directly calculated through the profile data of lncRNA, miRNA, and mRNA by the threshold of correlation coefficients.
Integrated databases can be used to filter calculation outcomes to obtain more reliable pathways. Moreover, opplncRNA has the functionality of directly demonstrating 3 layers network from lncRNA to mRNA in command line form. 3) oppHeatmap, which is preferred visualization modes for biologists to display high-dimensional information from high-throughput omics data. Many software including website services and R packages are available to generate various types of customized heatmaps.

oppHeatmap is another choice for rendering different kinds of heatmaps through MATLAB. It is available for plotting ordinary heatmaps, hierarchical clustering, TreeMaps, microplates graph, sample correlation, gene correlation, and polar heatmaps. It can support the modification of borders, fonts, and colors to customize the final plots. It can not only read data from Microsoft Excel to generate specific heatmaps but also make Excel heatmaps by coloring each cell in Excel. The graphs can be stored in supported vector graph (SVG) format and modified by other SVG recognition software. Therefore the intregrated opp omics pilot platform named oppStudio was constructed under a serie of modules, including oppDNA, oppRNA, oppProtein, opp-miRNA,opp-circRNA, ,oppMetabolism, oppSingleCell, oppWB, and other. The GUI of above modules are all developed based on the architecture of AppDesigner in MATLAB, and all input and output files from Microsoft Excel. It is independently easy-to-use and can be read and calculated directly for omics data analysis.

Improved Estimation of Material Parameters for Cardiac Modelling Using Deep Neural Networks

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Cardiovascular disease is the leading cause of mortality worldwide, accounting for approximately one-third of all deaths. Biomechanical modeling of the heart based on personalized medical images has immense potential for enabling precise diagnosis of cardiac diseases. The stress distribution within the myocardium is closely related to the left ventricular ejection function and heart disease development. However, accurate stress estimation relies on inferring material parameters from cardiac motion, an inverse problem in mathematics. Traditional optimization schemes require numerous iterations to match simulation results to medical image observations, which is computationally expensive. In this study, we explored using a convolutional neural network (CNN) to estimate cardiac material parameters, accelerating the optimization process. First, we adopted the Holzapfel-Gasser-Ogden (HGO) constitutive model to characterize the myocardium's hyperelastic and anisotropic material properties[1]. The strain energy function contains 8 material parameters. To reduce the high-dimensional estimation difficulty, we divided the 8 parameters into 2 groups and simplified them to 2 coefficients and based on prior material tests. Next, we reconstructed the left ventricle's undeformed structure (zero pressure) at mid-diastole from magnetic resonance images of 20 volunteers. We simulated the myocardium's deformation and obtained the deformed structure under physiological pressure with different material property combinations. This resulted in a dataset of 2000 cases, with each case containing the undeformed and deformed shapes and corresponding <Ca, Cb> labels. We split the dataset into training (1200 cases), validation (300 cases), and test (500 cases) sets at the volunteer level. We trained a ResNet18 to rapidly estimate cardiac material parameters from the undeformed and deformed structures. Specifically, we used the middle-ventricle segmentation mask as input and the corresponding <Ca, Cb> as output, with mean absolute error (MAE) as the loss function. The experimental results show that the average absolute errors of the two parameters are 0.252 and 0.316 respectively. Furthermore, we used the ResNet18 predicted values as initial values for the traditional optimization methods to achieve faster convergence, achieving 10x acceleration. In conclusion, the feasibility of using deep neural networks to estimate cardiac material parameters is validated, which can be applied to accelerate patient-specific cardiac modeling and has the potential for clinical translation.

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A condition monitoring methodology using machine learning with parameter discovery applied to heat pumps

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A recent review of condition monitoring using machine learning [1] shows that different techniques are applied for fault detection, classification, location, and quantification. These approaches are typically data-driven or model-based, with the latter challenged by experimental uncertainties and modelling errors [2]. Here, model-based often refers to the estimation of unmeasurable state variables in a dynamic system, with the traditional approach being the Kalman Filter or variants thereof. However, in some cases models are based on fundamental physics. Using these physics-based models usually involves direct comparison between actual measurements and model predictions and considering the residuals as fault indicators. This usually works well for fault detection, but not necessarily for classification and isolation [2]. Another approach is to monitor the rate of change of specific key parameters within the physics-based model via parameter discovery to detect potential faults [3]. In this paper we propose the use of a fundamental physics-based thermofluid model of a heat pump cycle combined with parameter discovery and deep neural networks to simultaneously detect, locate, and quantify degradation occurring in the different heat pump system components. The concepts are demonstrated with the aid of synthetic measured data generated via simulation. The physics-based model is first calibrated by discovering specific values that characterize the component model behavior, including geometrical parameters, empirical coefficients, and operating parameters. The calibrated physics-based model is then used directly with parameter discovery to pinpoint and quantify performance degradation. Alternatively, the calibrated model is used to generate synthetic performance data while postulating values for degradation factors applied to specific component characteristics. This data is used to train deep neural networks that are then used either directly or in conjunction with parameter discovery. A comparison is made between the different approaches in terms of required computational resources, accuracy, and sensitivity to experimental uncertainties and modelling errors.

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16. Discretization Methods, Grid, Mesh and Solid Generation

High-Order Mesh rp-adaptivity for Surface Alignment with Implicit Geometries

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Computational analyses with the finite element method typically requires geometrically accurate meshes. It is well know that high-order meshes can accurately capture curvilinear surfaces with fewer degrees of freedom in comparison to low-order meshes. Existing techniques for high-order mesh generation typically output meshes with same polynomial order for all elements. However, high order elements away from curvilinear boundaries or interfaces increase the computational cost of the simulation without increasing geometric accuracy. In prior work (Barrera et al., Knupp et al.), we have presented one such approach for generating body-fitted constant-order meshes that takes a given mesh and morphs it to align with the surface of interest prescribed as the zero isocontour of a level-set function. We extend this method to generate mixed-order meshes such that curvilinear surfaces of the domain are discretized with high-order elements, and low-order elements are used elsewhere. Using various numerical experiments, we demonstrate the robustness of the approach and show that it can be used to generate a mixed-order mesh that is much more efficient than a high constant-order mesh. The proposed approach is purely algebraic, and extends to different types of elements (quadrilaterals/triangles/tetrahedron/hexahedra) in two- and three-dimension.

Adaptive mesh refinement and coarsening procedures for the virtual element method

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The virtual element method (VEM) is a recent extension of the finite element method that permits arbitrary polygonal element geometry in two dimensions. This mesh flexibility means that the VEM is well-suited to problems involving adaptive mesh refinement. However, the VEM 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 simple Z2-based error estimator has been implemented using a super-convergent patch recovery procedure. Using this error estimator elements are flagged for refinement or coarsening. The refinement [1] and coarsening [2] of the elements is performed using novel remeshing procedures that are suitable for the arbitrary polygonal element geometries permitted by the VEM. The remeshing procedures have been implemented for the VEM for the case of two-dimensional elastic problems. The procedures are motivated by seeking to reduce the global error approximation and to improve/smooth the error distribution over a problem domain to improve the efficiency of the VEM approximation. The performance of the remeshing procedures has been investigated in terms of accuracy in the H1 error norm with respect to computational cost and is compared to a traditional reference uniform mesh refinement procedure. Numerical results over a wide range of benchmark problems demonstrate that the proposed remeshing procedures represent significant improvements in computational efficiency. Specifically, the adaptive refinement procedure generates solutions of equivalent accuracy to the reference procedure while using significantly fewer degrees of freedom, and significantly less run time. While the adaptive coarsening procedure can generate meshes comprising significantly fewer degrees of freedom compared to uniform meshes while introducing only a small amount of error into the approximation.

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A Weakly-Compressible Two-Phase Formulation for Hydrogen Containment Modelling

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The design of cryogenic storage tanks rely on the accurate modelling of the self-pressurisation and sloshing process which occur during the storage and transportation of liquefied gases at extreme low temperatures. In this context, an accurate and efficient weakly-compressible Volume-of-Fluid (VoF) model based on the two-fluid formulation proposed by Baer & Nunziato [1] is developed and simplified via a non-dimensional analysis of a liquid-gas hydrogen system at saturation conditions. The resulting model treats the liquid as incompressible and the gas as compressible. The set of governing equations are solved via the implicit pressure based projection method in Elemental ® [2, 3, 4] which is extended to include non-isothermal effects.
Unlike traditional compressible flow solvers which employ a two-way coupled system for pressure and temperature, an implicit pressure solve is found sufficient and superbly efficient in capturing both sonic characteristics and thermal effects in the gaseous phase. The model is validated using academic and industrial relevant test-cases. These include a syringe problem to validate compressibility effects, a natural buoyancy case to validate non-isothermal effects and a classic flight-weight case [5, 6] to demonstrate the ability of the model to capture pressurisation for liquid-gas hydrogen. For all tested cases, an excellent correlation is seen between analytical and numerical solution. We also focus on a two-phase mass inflow pressurisation which is subjected to a violent acceleration. In particular, the results show flow features consistent with that obtained in literature where the developed solver is found to be both accurate and efficient for such industrial relevant problems.

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17. Flow Problems

Inlet waveform effects on non-Newtonian flow through stenosed arteries

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In numerical hemodynamics research blood is usually modelled as a Newtonian fluid while the inlet waveform is usually modelled as a sine wave, even though blood has been shown to exhibit shearthinning and viscoelastic properties, and it is known that physiological waveforms differ significantly from the sine wave. Research into the combined impact of both effects on flow behaviour has been sparse.
Considering the significant variation in real-world arterial waveforms, assessing how different features, such as amplitude, asymmetry and pulse duration impact the flow field is beneficial. Similarly, there is no consensus on which non-Newtonian model to use when modelling blood. Models differ in their complexity and computational cost and degrade both numerical stability and convergence rate, so it would be advantageous to use the simplest one capable of accurately capturing flow behaviour. Both of these effects complicate Reynolds number computation which in turn impedes accurate comparison of different numerical and experimental data, hence a robust way of computing the bulk Reynolds number is also necessary.
Given the outlined problems, it is the aim of this work to numerically investigate the impact of physiological waveforms on the non-Newtonian flow through an idealised, axisymmetric stenosed artery. A parametric study is performed to assess the effects of different inlet waveforms and rheological fluid models. Real-world physiological waveforms in conjunction with several rheological fluid models, fitted to whole-blood data, are used in numerical flow simulations employing the cell-centered finite volume method. The simulations are run for several Reynolds numbers and stenosis intensities.
Key flow features are compared against benchmark cases and experimental data available in the literature. An assessment of rheological models and suitable bulk Reynolds numbers computation methods is made based on the results.
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A new implicit fan model for robust air-side heat exchanger simulation

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Actuator-disk fan models are widespread in industrial cooling fan literature; however, their ability to accurately assess fan performance over a wide range of operating conditions has been historically limited. Actuator-disk models implicitly represent the rotor of a turbomachine as a momentum source where the source term strength is determined from two-dimensional (2D) blade-element force calculations. These force calculations are typically completed using standard 2D airfoil coefficient input data. However, conventional 2D airfoil coefficients limit the usable range of the models to only near-design machine operating conditions, where the flow over the rotor itself is principally 2D. At off-design flow conditions, the flow regime over the rotor gains tridimensionality and the 2D coefficients

start to lose application, constraining the models' accuracy. Unfortunately, off-design operating conditions are unavoidable in many industrial heat exchanger systems, so the limited off-design performance of actuator-disk fan models is a concern.
A new means of determining appropriate model input coefficients, purpose-built for low-pressure axial flow fan analysis, has thus been developed. The Augmented Actuator-Disk Method (AADM) has been shown to accurately predict fan performance and fan blade loading over a wide range of operating conditions. The AADM has also been somewhat shown to better predict physical fan flow profiles. This improved flow field resolution of the AADM is a potentially key feature in the context of industrial heat exchanger studies (where air-side flow characteristics have a distinct effect on system effectiveness) and further assessment of this capability is warranted. This study, therefore, further explores and quantifies the accuracy of the new AADM's resolved flow fields using computational fluid dynamic (CFD) simulations. The accuracy of the AADM's flow fields is quantified relative to equivalent explicit (full rotating fan geometry) fan model computations and compared to other current actuator-disk fan model variants. Consistent with the initial indications, the AADM's improved off-design flow field resolution is confirmed, establishing it as a valuable tool for future industrial heat exchanger research.

Numerical Simulation of Laminar and Transitional Flow and Heat Transfer for a Wavy-finned Flat-tube Heat Exchanger

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Wavy-finned, flat tube heat exchangers are used in industrial heat exchangers due to their relatively low frictional pressure drops and high heat transfer coefficients (Bonger, 1994). Originally developed for mechanical draft systems, these heat exchangers are now finding application in natural draft (buoyancy driven) systems (e.g. in natural draft direct air-cooled condensers). In the context of these natural draft systems, careful consideration of tube configuration (notably fin configuration) is warranted due to the juxtaposition of pressure drop (resistance) and heat transfer coefficient (which contributes to motive potential) in these tubes and the sensitivity of the overall system performance to these parameters. This work forms part of a larger study which aims to optimize wavy-finned, flat tube heat exchanger configuration for natural draft direct air-cooled condenser application. A first step in this process involves the generation of a validated tube model and the evaluation of the applicability of existing analytical / empirical models for a wide range of tube parameters. Numerical studies of wavy-finned, flat tube performance have been conducted for fully laminar flow (e.g. Duan et al. (2016)) or for a wider range of flow (encompassing laminar and turbulent flow regimes) but using Reynolds-Averaged Navier-Stokes models such as the and formulations, which show a marked decrease in accuracy outside of the turbulent flow regime (Li, Du, Yang, Xu & Yang, 2013). This study presents a three-dimensional computational fluid dynamics model, employing the transitional SST turbulence model, for predicting tube performance in the laminar and transitional flow regimes. The numerical results are validated against experimental data and shown to correlate well over the full flow range considered (Reynolds numbers of 450 to 2300). The validated model is then used to assess the validity of existing analytical and empirical models for wavy-finned tubes for a range of tube parameters.

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Comparative Analysis of Lubrication Approximation and SPH-DEM Coupled Simulations for Rotating Drum Flows

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In this study, we present a novel approach to evaluate the efficacy of the lubrication approximation in comparison with SPH-DEM (Smoothed Particle Hydrodynamics-Discrete Element Method) coupled simulations for modelling rotating drum flows. SPH, renowned for its computational demands, has earned recognition for its exceptional ability to replicate complex fluid behaviour in free surface flows (eg. Splashing). Conversely, the lubrication approximation excels in scenarios characterised by dense granular systems wherein thin liquid films are prevalent. In the present study, the objective is to achieve statistical agreement between simulation results and in-situ measured data obtained through positron emission particle tracking experiments of rotating, dense granular flows. The system under investigation involves glass beads as the discrete solid phase simulated using DEM, while a water-glycerol mixture is represented by either SPH elements or the lubrication approximation, simulating liquid bridge induced forces. PEPT measurements offer an exceptional advantage with their impressive spatial and temporal resolutions, reaching down to the millimetre and millisecond scales, respectively. This level of precision allows for an exceptionally high fidelity comparison between our computational models and the actual physical behaviour of the rotating drum system. The evaluation metric thereof encompasses solids fraction, velocity fields and the emergent free surface. By adopting a mesoscale perspective using appropriately sized representative volume elements, we facilitate an in-depth analysis of the system's behaviour under different critical speeds and flow regimes. To our knowledge, this study marks a significant departure from conventional approaches. While studies involving SPH-DEM simulations and lubrication approximations have been conducted, the benchmarking against in-situ, high resolution experimental data and the assessment of the emergent free surface remain relatively unexplored areas. The potential insights from this study not only advance the understanding of rotating drum flows but also contribute to refining and calibrating the SPH-DEM coupled simulations and lubrication approximation models.

Simulating blood flow through pathological aortic valves using reduced order modelling, 3D CFD simulation and experimental approaches

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Aortic stenosis (AS) is a type of valvular heart disease (VHD) resulting in an inadequately opened aortic valve. This pathological condition is often a result of congenital malformation, infection, or degeneration due to ageing. Rheumatic heart disease (RHD), caused by rheumatic fever, results in a type of valvular stenosis. Worldwide, RHD is considered the most frequent cause of primary VHD where up to 40 million people were affected in 2019 with an incidence of over 2 million per year. In low and middle-income countries the disease accounts for more than 300, 000 deaths in 2019. Sub-Saharan African countries are of the few with the highest prevalence of RHD and associated mortality where the second leading cause of death in South Africa is VHD. Accurate diagnosis of the type and severity of valve lesion dictates both the urgency of medical intervention and patient prognosis. Diagnosis is often confirmed by evaluating patient symptoms, valve anatomy and valve

haemodynamics through medical imaging modalities or cardiac catheterization. Using Doppler echocardiography, the peak transvalvular velocity is measured and, in turn, utilized to calculate the mean pressure gradient by applying the simplified Bernoulli equation and a standard empirical modification. Literature suggests that the use of imaging data and the simplified Bernoulli equation to determine the type and severity of valve lesions over-simplifies the flow environment resulting under-estimated pressure gradients [1]. In this work, pressure gradients across generic aortic heart valves for varying degrees of stenosis and morphology type are measured using a simplified steady-flow test bench and 3D-printed valve geometries in full or restricted open positions. The experimental measurements for varying flow rates are in turn compared to values calculated using the standard clinical approach, more sophisticated empirical models accounting for fluid friction and expansion, and 3D computational fluid dynamics (CFD) models. The goal of the work is to investigate the differences between the experimental values for pressure gradient and previously mentioned model predictions. Through these simulations, an improved understanding of the effect of aortic valve stenosis morphology and severity on the haemodynamic and clinical parameters influencing diagnostic thresholds and cardiovascular disease prognoses will be developed.

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Numerical Modelling of Blood Flow During Syringing

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Hemolysis, defined as the breaking open of red blood cells, can occur due to a range of factors which can be physical, chemical or biological in nature. Physical damage can manifest in scenarios such as emergency rapid blood transfusions conducted through syringing, a practice which may be employed in resuscitation procedures, particularly in rural hospitals. It has been demonstrated that such syringe-based transfusions result in noteworthy hemolysis, significantly surpassing the impact of pressure bag usage. This heightened hemolysis carries potential negative implications for the recipient of the transfusion [1]. The core objective of this project revolves around emulating the blood flow through a sudden contraction, simulating a syringe, to emulate and quantify the underlying mechanisms driving hemolysis. Employing numerical simulations alongside a variety of hemolysis models [2], the goal is to identify the specific flow conditions that are most conducive to hemolysis occurrence. The modelling process commences with the depiction of blood flow as a Newtonian fluid traversing a sudden contraction, representing the syringe's action. This initial setup is subsequently expanded to account for non-Newtonian flow behaviours [3]. To validate the modelling approach, a two-dimensional scenario is first simulated using the finite element software deal.II. This is then repeated and compared to results from numerical simulations using ANSYS Fluent. The scope extends further to encompass a three-dimensional setup, incorporating a representative syringe and hypodermic needle. The time history of shear stress along streamlines is then extracted to facilitate hemolysis analysis.

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18. Transport Phenomena in Micro/nanofluids

Dynamics of a charged particle in a spherical cavity

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Dynamics of a charged particle confined in a spherical cavity were studied numerically. We calculated the forces acting on the particle at various locations in the confined space. The main force comes from the induced charges on the cavity wall. Several different dielectric permittivities are tested, and the magnitude of electric forces are calculated as the dielectric contrast changes. Under the influence of both hydrodynamic force and the force from electrostatic interaction, the charged particle's motion is very difference from non-charged case. This work forms the basis to understand more complex dynamics in microfluidic applications such as intracellular transport and encapsulation technologies.

Magnetized mixed convective flow of radiative fourth-grade tetra-hybrid nanomaterial over a horizontal cylindrical surface

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In this article, we investigate magnetized mixed convective flow and heat transfer scrutiny of nonlinear radiative fourth-grade tetra-hybrid nanomaterial through a horizontal circular cylinder with variable fluid properties, suction/injection and convective heat conditions at the surface. Tiwari–Das model has been utilized in the construction of the nanofluid model. Thermal transport evolution is characterized with the help of heat source/sink, viscous dissipation and Joule heating. The governing partial differential equations are first converted into dimensionless form using appropriate similarity transformations, and then solved numerically by means of the overlapping multi-domain spectral collocation method that uses local linearization approach. Numerical results that simulate the impressions of key parameters on flow quantities, wall frictional factor and heat transmission rate are computed, discussed and analyzed. In view of the obtained results, fluid flow is accelerated by material parameters and reduced by variable viscosity parameter, and the opposite is true for the skin friction factor. The use of tetra-hybrid nanofluid along with the inclusion of nonlinear radiation, heat source and variable thermal conductivity are important for thermal transfer enhancement. The rate of heat transport is enhanced with growing Biot number, nonlinear radiation, heat sink and variable thermal conductivity. The considered flow problem finds relevance in thermal performance enhancement of the working fluid, and polymer manufacturing procedures in chemical engineering.

Particle dynamics in a low-Reynolds-number fluid between two spherical shells

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Dynamics of a particle and the suspending low-Reynolds-number fluid confined between two spherical shells were studied numerically. We calculated the particle’s hydrodynamic mobilities at various locations in the confined space. The mobility is largest near the middle of confined space along radial direction and decays as the particle becomes closer to no-slip walls. Fluid vortices in the confined space induced by the particle motion were observed and analyzed. We also found that the particle can exhibit a drift motion perpendicular to the external force. Magnitude of the drift velocity normalized by the velocity along the direction of the external force depends on particle location and particle-to-

cavity sizes ratio. This work forms the basis to understand more complex dynamics in microfluidic applications such as intracellular transport and encapsulation technologies.

Transport of room-temperature ionic liquids under external electric fields in confined and unconfined spaces

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Room-temperature ionic liquids (RTILs) are promising electrolytes that are composed entirely of ions but are liquid at room temperature. Their remarkable properties such as wide electrochemical window, excellent thermal stability, and low vapor pressure make them ideal electrolytes in many applications such as supercapacitors, batteries, and electrospray devices. Here, by using molecular dynamics simulations, we explore transport phenomena of RTILs in confined and unconfined spaces. In the confined space, electroosmotic flow, ionic transport through nanopores, and charging kinetics of RTILs between parallel plates were studied. In the unconfined space, interfacial ionic transport across the RTIL-vacuum interface was investigated. Fundamental understanding obtained in these works will lay the foundation to improve theoretical modeling of RTILs and also the performance of applications utilizing RTILs.

Simulations of particulate transport in low-Reynolds-number fluids confined by general geometries

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A parallel Stokes' solver has been developed for description of hydrodynamic interactions between particles in low-Reynolds-number fluids confined by general geometries. A Langevin description of the particle dynamics is adopted, where the long-range interactions are included using a Green's function formalism. A scalable parallel computational approach is presented, where the general geometry Stokeslet is calculated following a matrix-free algorithm using the general geometry Ewald-like method. Our approach employs a finite-element Stokes' solver for the accurate treatment of long-range hydrodynamic interactions in arbitrary confined geometries. The method is a combination of mid-point time integration of the Brownian stochastic differential equation, the parallel Stokes' solver, and a Chebyshev polynomial approximation for the fluctuation-dissipation theorem.
We illustrate the new solver in the context of the dynamics of confined polymer solutions under equilibrium and non-equilibrium conditions. The method is then extended to treat suspended finite size particles of arbitrary shape in any geometry.

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