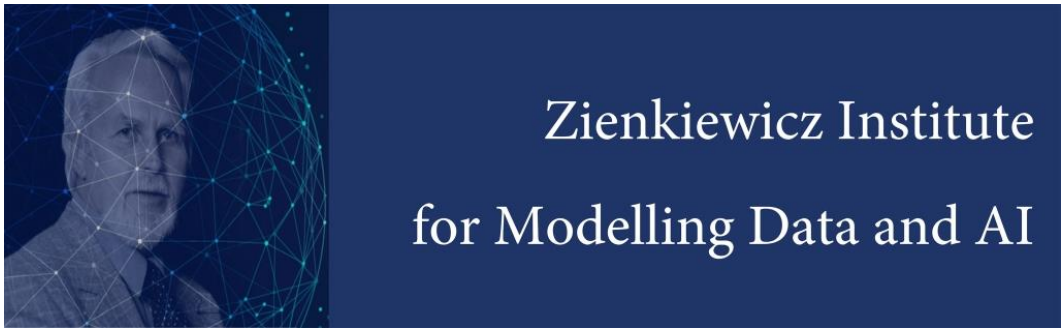
Eccomas Thematic Conference

Computational Methods in Multi-scale, Multi-uncertainty and Multi-physics Problems

CM^{4}P 11 September – 13 September 2023, Porto, PortugaL



ABSTRACTS PROCEEDINGS

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Tri-phase Simulation of Cavitating Flow with Discrete Particles

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Metal additive manufacturing (A.M.) has enabled the ability to produce complex component geometries. Such A.M. techniques, however, create rough surfaces and require further enhancement to reduce crack initiation spots that lead to devolved fatigue performance [1, 2]. Hydrodynamic Cavitation Abrasive Finishing (HCAF) is one such process developed to finish additively manufactured internal surfaces utilizing synergistic effects between particle abrasion and cavitation erosion [3] to achieve good surface finish. This finishing process is currently under exploration for extending its application towards external surfaces. A multi-jet nozzle (see Fig 1) that includes a slurry (water + abrasives) flow enveloping a high-pressure cavitation flow is used to investigate the effects of HCAF on external surfaces. Since observations of the nozzle's internal flow and the outflow field (the slurry is highly opaque) are impossible, there is a need for modeling this new HCAF application numerically for predictions, visualization, and parametric investigations.

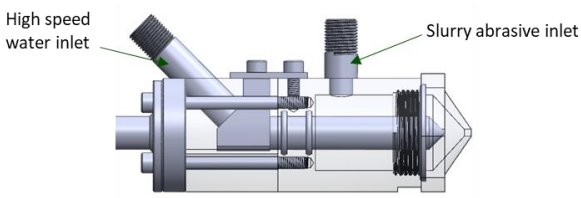

Figure 1. The multi-jet nozzle for external HCAF usage

Although simulations of the HCAF's cavitating aspect have been done in internal channel, wall-bounded flows [4], there has been no attempts on combining the cavitation aspect with the abrasive aspect. As this HCAF's application is a new topic, the possible modeling setup is also unknown as the tri-phase, multiple-region-flow that transitions from wall-bound to an almost free-field region is complex, and very unlike previous applications. This research study attempts to produce a numerically stable model of the external HCAF process in the commercial

ANSYS Fluent software (2021 R2) as part of developmental efforts and serves as a primer to simulating cavitating flows with discrete particles.

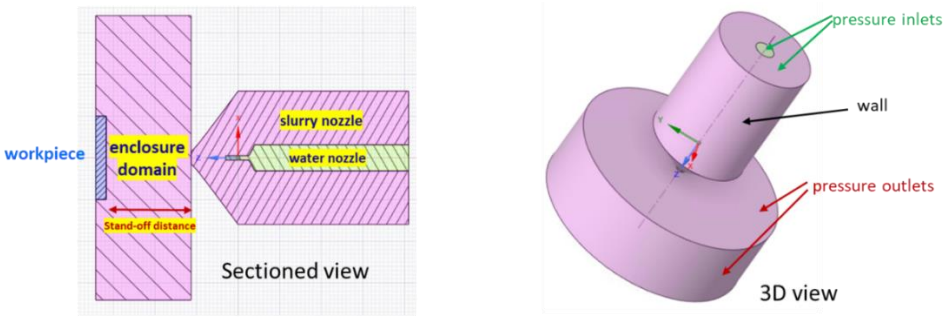

Figure 2. Sectional view (left) and 3D view (right) of the fully constructed fluid domain model

A simplified model of the nozzle is first drawn using CAD software before combining it with a target sample workpiece with the prescribed stand-off distance (see Fig 2). An enclosure is then made to serve as the fluid domain between the nozzle and the workpiece. Pressure inlets and outlets are defined and illustrated as shown in Fig 2. To model the tri-phase nature of the process, both Eulerian and Lagrangian methods of phase tracking are employed for the cavitation bubbles and abrasive particles respectively. The water liquid-vapor mass transfer (cavitation) is described by Schnerr-Sauer's model. The Volume of Fluid (VoF) model is employed to simulate liquid-vapor continuity along the fluid domain. Silicon carbide particles are injected through the slurry inlet at 1% of the water flow rate with the Discrete Phase Modeling (DPM) feature to model the abrasive slurry concentration. Turbulence is modelled with the k-ω SST model to account for the close-wall interactions within the nozzle. The flow field is initialized first with only the turbulence model before incorporating cavitation and DPM for convergence stability. The final flow field and output contours are then discussed to understand the model's viability as an evaluation tool for process parameters and nozzle design. The outputs of modeling are used to explain the effects of input parameters, flow visualization, and for predicting the efficacy of different input combinations. Nevertheless, further work could be done on the scenes of erosion modeling, and multiphase interaction models for improving this tri-phase model's comprehensiveness.

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Phase-field modelling for drying-induced cracks:
from homogeneous to localized damage

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A phase-field model has demonstrated its effectiveness in addressing drying-induced crack phenomena in soil [1-3]. In this study, we delve into specific fundamental aspects of the model to achieve a deeper mathematical understanding. First, we compare two prevalent models in which the damage is coupled with either the effective or the total stress. This comparison is based on their performance under two benchmark setups: free and restrained desiccation. Through this evaluation, we aim to identify the model that yields more reasonable results. Subsequently, we conduct a semi-analytical computation of the damage evolution for the selected model. The results reveal that, in a restrained desiccation setup, the damage is initially homogenous and then bifurcates into a periodic solution, resulting in damage localization. Moreover, key information such as the first bifurcation time and the crack spacing is also derived as a function of material and loading parameters. Finally, to validate the analytical findings, we solve several numerical examples using the Finite Element Method (FEM), which demonstrates good agreement between the analytical and numerical results.

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Explicit Formulation of Adiabatic Viscoplastic Johnson-Cook Type Constitutive Models

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This study presents an explicit formulation that is analytically derived from the well-known adiabatic viscoplastic Johnson-Cook (JC) implicit model. It has been found that the explicit formulation can be considered as a new independent constitutive material model with insights that are not observed from the classical implicit JC model. The proposed explicit model led to a new material parameter that lumps other material parameters and can be determined from experimental results. The coupling of the strain and strain-rate hardening effects with thermal softening effect is clearly reflected in the explicit model and offers a better understanding of the thermo-viscoplastic material flow. Furthermore, the efficiency, accuracy and numerical stability of the proposed explicit model had been numerically tested by simulations of two well-known bench-mark time dependent problems, that are characterized with high impact loading and high strain-rate. To validate the proposed explicit constitutive model an external UMAT subroutine has been encoded and imported in ABAQUS\CAE 6.14 software. It has been found that numerical results of finite element simulations associated with the proposed explicit model are in excellent agreement with the numerical results of simulations associated with the classical implicit JC model, and with experimental data. In addition, it has been found that numerical simulations of adiabatic thermo-viscoplastic response are numerically more stable and more efficient when executed with the proposed explicit model.

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A Case Study to Validate Drag Models by ANSYS Fluent and CFD-DEM Simulation

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There are a very wide variety of drag models available while there is not yet a clear outcome on which is the best performing model. This is because the various models all perform differently under different operating conditions. With new drag models (or drag model enhancements) being regularly updated, drag models are categorised into three main groups based on their derivations: experimental, Lattice-Boltzmann simulations and numerical simulations.

There are many other drag models which fall into these categories. These will be discussed in the study, although not all of them were simulated. Instead two examples of each category will be discussed. These have been chosen for their reliability and common use in literature. They are Gidaspow model and Rong et al model for experimental category, Hill-Koch model and Beestra et al model for Lattice-Boltzmann simulations category, and Teeneti model and Symlal O'Brien model for numerical simulations category.

In this study, a L-shape box was created as a test case to assess these drag models. Two types of simulations, ANSYS Fluent simulation with fixed-location particles and CFD-DEM simulation with moving particles, were performed to draw conclusions independently, and comparison between them can evaluate accuracy of CFD and CFD-DEM simulations. In CFD simulation which is done by ANSYS Fluent, a number of particles are set in the joint part to form a porous area and the space of these particles are set as void so that a pure fluid field is accessed. CFD-DEM simulation was conducted with a in-house code. Both simulations draw a conclusion about the performance of different models for this particular L-shape box case. While the overall performance for other cases needs to be studied further.

A Finite Element-Boundary Element Coupling Method for Elastoplastic Analysis of Multiscale Structures in Electronic Packaging

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The electronic packaging plays the key role of support and protection in integrated circuits. With the rapid development of advanced electronic system, increasing research has been made to enhance the reliability of electronic packaging. During the operation of electronic devices, a high amount of heat will be generated due to the resistance to the current transmitted through the transistors, thus generating a significant temperature gradient on each packaged component. The presence of temperature gradient can cause many problems in an electronic system such as thermal migration, solder joint failure, chip failure etc. Therefore, long lasting packaging reliability is one of the key requirements for the design and development of electronic packaging structures.

With characteristics of easy implementation, resource saving and less environmental restriction, the simulation-based design for electronic packaging structures is currently a mainstream technique. At present, various programs, focused on mechanics reliability analysis, mainly based on the FEM, are available, i.e., ABAQUS, ANSYS, COMSOL. However, due to the multiscale structures in the electronic packaging, numerical model requires very fine discretization with large number of degrees of freedom to ensure the computational accuracy, which is computational undesirable. To address this issue, the boundary element method is extended and used to analyze electronic packaging problems.

In the present talk, we will introduce a FE-BE coupling scheme to analyze mechanical problems in electronic packaging. Since the user element implementation in the ABAQUS permits the element to function in a way like any standard ABAQUS finite element, the boundary element region is treated as a ‘finite element’ and incorporated into ABAQUS by UEL. The benefits of proposed method are: (i) the powerful pre- and postprocessing of ABAQUS; (ii) the higher accuracy of the solution; (iii) the less computational cost and higher efficiency.

Multiphase flow

A numerical model for heat transfer coefficient in flow boiling and condensation in a horizontal straight tube with zeotropic mixtures

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This work presents a numerical study on the boiling and condensation of zeotropic mixtures in Joule-Thomson (JT) refrigeration cycles applied in cryogenics. Zeotropic mixtures never have the same liquid and vapor composition in the liquid-vapor equilibrium. Additionally, they exhibit a separation between the bubble and dew point, known as the glide temperature (T_{glide}). These characteristics make zeotropic mixtures suitable for JT refrigeration cycles, significantly improving their performance. JT cycle optimization has gained substantial importance in cryogenics applications, including gas liquefaction, cryosurgery probes, cooling of infrared sensors, cryopreservation, and biomedical samples. Moreover, zeotropic mixtures have proven effective as working fluids in organic Rankine cycles, especially those utilizing fourth-generation heat transfer fluids.

The design of heat exchangers for these cycles is critical, particularly regarding the heat transfer coefficient and pressure drop of two-phase zeotropic mixtures. In this study, a comprehensive methodology is applied to calculate local convective heat transfer coefficients based on the law of the wall approach for turbulent flows. Numerical investigations are carried out for zeotropic mixtures in horizontal tubes, analyzing pressure drop, temperature profiles, and heat transfer coefficients for mixtures of different compositions. The numerical model is locally applied to fully developed, constant temperature walls, and two-phase annular flow in ducts. Results are obtained by solving continuity, momentum, and energy equations. Local heat transfer coefficient results are compared with experimental data published by Nellis et al. (2005), Barraza et al. (2016), and Maarak (2009), demonstrating good agreement.

Solving Multiphase Flow Problems using Intelligent Finite Element Methods

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Abstract

During the last three years, artificial intelligence (AI) has provided the ability to address challenges that could not be resolved by classical means, such as the identification of images and autonomous vehicles. Recently, we have been instrumental in developing a new approach to solving Partial Differential Equations (PDEs) using AI libraries [1,2,3]. This work has not only made the algorithms, based on these libraries, highly efficient and portable between different computing architectures, but has substantially simplified the implementation of the numerical methods to solve flow dynamics. In this work, we present a novel AI-based methodology to bring the power of AI software and hardware into the field of multiphase flow problems. Convolutional Neural Networks (CNNs) are formed by the most popular AI libraries, Pytorch and Tensorflow, in order to solve the incompressible flow equations on structured mesh through a finite element discretization and a rapid multi-grid solution method. Volume of Fluid (VoF) and compressive advection approach are implemented in the neural networks to accurately capture the interface between different phases. The presented AI high-fidelity solver is applied to predict complex multiphase flows such as air bubble, water droplet, collapsing water column and slug flow within a pipe. The results are validated with previous studies [4,5] and indicate that the new method can solve all those problems in an effective way.

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Study on the Influence of Carbon Nanotubes on the Mechanical Behavior of a Cementitious Matrix Using Computational Homogenization

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In this work, the application of carbon nanotubes (CNT) as reinforcement for a cementitious matrix is studied. To achieve this, a multiscale numerical framework is developed in MATLAB and coupled with the finite element software ANSYS Mechanical. This framework enables the simulation of the mechanical properties of the CNT+cement composite, taking into account the properties of the CNTs, the cementitious matrix, and their interphases. The framework incorporates atomistic simulations of the CNTs (García-Macías et al., 2019), using a finite element structural approach, as well as computational homogenization of the cementitious matrix (García-Macías et al., 2018). The interphase between the CNTs and the cement matrix is modeled using micromechanical approximations of a smooth interphase. Additionally, properties of the cementitious matrix such as moisture, porosity, and inclusion of particulate material are considered. The results highlight the significant influence of parameters such as CNT orientation, number of layers, and chirality on the mechanical behavior of the CNT+cement composite.

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Multi-Adaptive Framework for Computational Efficiency in Peridynamic Modeling: Applications in Material Science

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In this contribution, we introduce a multi-adaptive framework designed to enhance the computational performance of peridynamic (PD) models. Our approach synergistically combines a collocation-based meshfree discretization scheme with the classical standard scheme, while maintaining an emphasis on efficiency and accuracy. The innovative aspect of our method lies in the dynamic application of a less demanding quadrature and a multi-grid approach across the majority of the computational domain, reserving the more computationally demanding standard scheme for localized regions with discontinuities and material damage. A key efficiency feature of the proposed method is the adaptive adjustment of neighborhood node numbers. To demonstrate the practicality and effectiveness of our approach, we have evaluated its application to two distinct problems: the Kalthoff-Winkler experiment and the degradation of a magnesium-based bone implant screw. Our balanced approach to PD modeling not only curtails computational costs but also fulfills the requisite accuracy standards.

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Comparison of Hemodynamic Characteristics of Localized Aortic Valve Calcifications under Uniform and Helical LVOT Flows

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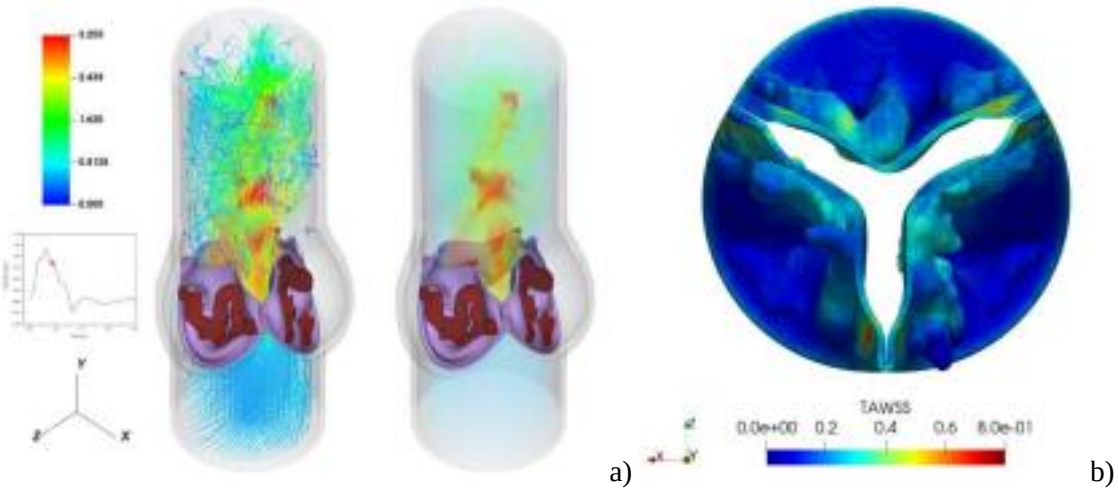
Blood rheology [1] has a critical role in both design process of patient-specific prosthetic heart valves, and identification and prediction of cardiovascular diseases. One of the most common valvular diseases is aortic stenosis (AS), which is caused by a reduction in the orifice area between the valve leaflets and leads to restriction of blood flow toward the body. Calcium build-up on leaflets plays a major role in the development of stenosis as calcium deposits increase the rigidity of the leaflets and hinder the functionality of the valve. Furthermore, the presence of non-uniform calcification patterns greatly affect the flow hemodynamics. AS can result in serious complications that may lead to mortality and morbidity in severe cases.

The motion and deformation of the localized calcified aortic valve leaflets as a result of coupled interaction between flexible tissue with calcium deposits and blood flow leads to a complex Fluid-Structure Interaction (FSI) problem. In order to create a realistic flow field around the aortic valve in terms of FSI modelling, it is crucial to define proper physiological boundary conditions, such as well-balanced LVOT (Left Ventricle Outflow Tract) flow rates accounting for AS based on corresponding calcification grades.

Although LVOT flow is almost uniform in most healthy cases, due to some LVOT disorders, LV (Left Ventricle) disfunctions, congenital anomalies and effect of AoSAs (Aortoseptal Angles), it is observed that helical LVOT flow interacting with aortic valve leaflets leads to significant flow disturbances, unpresidential leaflet stress distributions and dynamics.

The aim of this study is to examine the effects of localized calcium formations for several

grades on aortic valve leaflets under uniform and helical LVOT flow. To model the calcified aortic valve problem, we used IBFE (Immersed Boundary - Finite Element) method proposed by Griffith et al. [2]. FSI simulations of single-phase Newtonian blood flow under realistic boundary conditions are conducted, including helical inflow velocity profiles and an aortic outflow pressure represented by three-element Windkessel model. In order to quantify the critical parameters of blood flow and investigate the effect of calcification severity on the aortic valve functionality, numerous indexes based on transvalvular hemodynamics and Wall Shear Stress (WSS) are obtained. While energy loss, aortic jet velocity, kinetic energy and the average magnitude of the vorticity describe the transvalvular hemodynamics, WSS based indexes include TAWSS (Time averaged Wall Shear Stress), OSI (Oscillatory Shear Index), RRT (Relative Residence Time) and transWSS (Transverse Wall Shear Stress). Additionally, for the first time in the literature, the impact of right- and left-handed helical inflow from LVOT on aortic valve leaflets is analyzed and discussed with comprehensive indexes, including Helicity index and its intensity. Our initial results show a well-alignment with clinical observations (Figure 1).



a) b)

Figure 1: a) Streamlines and volume contours of velocity magnitude [m/s], b) TAWSS [Pa] distribution on severely calcified aortic valve leaflets.

ACKNOWLEDGEMENTS

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A Multiphase Finite Element Poro-Viscoelastic Model for Soft Biological Cells

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Soft biological cells, such as red blood cells and endothelial cells, exhibit intricate mechanical properties that arises from their complex composition and structure. Understanding and accurately modelling the mechanical behaviour of living cells has become a subject of utmost importance for a wide range of biomedical applications, including drug delivery, tissue engineering and medical image analysis.

In this study, we have developed a multicomponent finite element model (FEM) that incorporates the Cell Membrane that encloses the Cytoplasm and the Nucleus, located in the interior. The cytoplasm of soft cells exhibits both elastic and viscoelastic mechanical properties because of their deformable solid matrix, formed by organelles,
actin filaments and microtubules, which interacts with the entrapped cytosolic liquid (poromechanical coupling) [1], [2]. Provided that, the cytoplasmic space is represented as a biphasic material incorporating an incompressible visco-hyperelastic solid network (accounts for the actin and intermediate filaments) and a Newtonian incompressible fluid. The nucleus, on the other hand, apart from a nonlinear stress-strain relationship, exhibits also time-dependent phenomena [3]; therefore it is represented as a visco-hyperelastic material. At last, the cell membrane is modelled as a thin stiff hyperelastic layer. Our formulation is expressed in an arbitrary Lagrangian-Eulerian (ALE) framework, fixed to the solid matrix.

The cell is subjected to uniaxial tensile tests under different loading conditions including elongation, compression and loading/unloading cycles. The predictions of our numerical simulations are able to capture the key mechanical features of soft biological cells, such as the nonlinear stress-strain behaviour and the time-dependent viscoelastic response. Then, we examine the influence of various mechanical and viscoelastic properties in the tensile dynamics of the cell through a comprehensive parametric analysis.

This work is part of the Research Project "Multiscale modelling for the autoregulation

of Microvessels, CARE" which was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the "1st Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment" (Project No. 876)

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Structural properties of azopolymers for optoelectronic applications

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In recent decades, there has been a significant acceleration in the pace of development of modern technologies in the field of optoelectronics, photonics, and holographic techniques, resulting from the growing demand for efficient and cheap optoelectronic devices. One of the most promising photoactive materials, which are an alternative to commonly used inorganic compounds, are photochromic polymers. Particularly interesting are polyimides functionalized with azobenzene and azopyridine derivatives, called azopolymers. The photochromic mechanism in these materials is based on photoinduced trans-cis-trans isomerization. Irradiation of azopolymers with a polarized light can lead to dichroism, photoinduced birefringence, or macroscopic migrations of polymer chains forming surface relief gratings (SRG). These phenomena open up new possibilities for the use of azopolymers.

In the present work, the structural and thermodynamic properties of polyetherimides (ULTEM) with covalently anchored azochromophores ($Az(CH_2)6$-p-Py) forming the side groups of the polymer as well as dispersed in the polymer matrix at a concentration of 2 and 10 wt% were investigated using molecular dynamics (MD) methods. The MD simulations were performed using the GROMACS software applying the CVFF force field. The spatial distribution of chromophores in the polymer matrix was investigated using the intermolecular radial distribution (RDF) function. Analysis of conformational properties of all simulated azosystems was carried out. Moreover, the glass transition temperature was established and the phase transition processes were discussed. Was shown that the different topologies of polymer with covalently bounded and dispersed chromophores affect the thermodynamic parameters of the material. These properties will affect the electron and optical properties of the simulated azosystems giving effect in optoelectronic applications.

Investigation into the hygro-viscoelastic properties of fibre reinforced polymer composites via an asymptotic homogenization apporach

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The use and development of fibre reinforced polymer composites for engineering applications has increased its popularity in the last decades. Some of the characteristics that make this material attractive to the industry are its lightweight, high stiffness and an outstanding resistance to corrosion, moisture, and fatigue. Applications can be found in bridge engineering, aerospace structures, automotive and marine industries. One of the remaining concerns related to this type of composites is its hygro-mechanical response. The latter, very relevant in applications where the material is exposed to wet environments, in which humidity changes and water diffusion are present. Furthermore, under this scenario, the interaction between moisture diffusion and the viscoelastic nature of the composite needs to be accounted for. To tackle this issue, in this work an asymptotic homogenization-based approach is proposed to investigate the coupled hygro viscoelastic response of fibre reinforced polymer composites. First, the framework introduced in [1] is extended to hygro-viscoelasticity, where the time dependency is addressed by means of the correspondence principle [2,3]. The time domain equilibrium problem is transformed to the Laplace-Carson domain, where the viscoelastic equilibrium problem is solved as a fictitious elastic one. Once the effective properties are determined, they can be transformed back to the time domain. This strategy is used to investigate the hygro-viscoelastic response of fibre reinforced polymer composites. To this end, a two scale woven composite model, considering the yarn and woven scales, is proposed. The estimated effective macroscopic properties illustrate the predictive capabilities of the model and capture the time dependent nature of its hygro-mechanical properties.

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Homogenized descriptions for the elastoplastic response of polycrystalline solids: mean-field approximations vs. full-field simulations for neutron-irradiated bainitic steels

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Nuclear reactor pressure vessels are mainly made of bainitic steels. These steels can undergo microstructural changes due to the neutron radiation that impact their elastoplastic response and concomitant fracture toughness. Crystal plasticity laws have been recently proposed that express microscopic plastic slip rates within crystals in terms of key microstructural features such as densities of forest dislocations, dislocations loops, and solute clusters. The laws encode information from lower length-scale simulations generated by molecular and dislocation dynamics. Macroscopic elastoplastic deformations are determined here by homogenizing such crystal plasticity laws via mean-field approximations and full-field simulations. Mean-field approximations are generated employing various schemes of increasing complexity such as the elementary schemes of Taylor and Sachs or the more recent self-consistent schemes based on the concept of linear-comparison media. Full-field simulations, in turn, are generated with a Fast Fourier Transform algorithm implemented in the computer code CraFT. Several ways of accounting for local hardening in the mean-field approximations are presented and discussed. Sample results are provided for untextured samples subject to uniaxial tension. The elementary schemes of Taylor and Sachs predict quantitatively different responses, while the so-called Fully Optimized Second-Order (FOSO) scheme and the full-field simulations predict very similar responses for both non-irradiated and irradiated samples. Similar agreement is found between

predictions for dislocation densities and their evolution with applied load. Overall, the FOSO scheme is found to provide the best compromise between precision and mathematical complexity to generate homogenized descriptions for the elastoplastic response of polycrystalline media governed by complex crystal plasticity laws.

Crossing scales in constitutive modeling of damage in elastomers Laura Moreno-Corrales [1], Miguel Ángel Sanz-Gómez [1], Francisco J. Montáns [1,2]

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The classical statistical theory of elastomers, used also in soft tissues, establishes the behavior of the macromolecule, which, after a suitable micro-macro connection, facilitates the overall behavior of the elastomer as a continuum. Traditionally, an affine connection is employed with respect to the orientation, which is in contradiction to the usual computational homogenization approach, which averages Piola stresses and Deformation gradients. We recently demonstrated that the orientationally non-affine full network integration facilitates a behavior consistent with experimental evidence, overcoming many of the contradictions in the theory of elastomers. We have demonstrated that with the new approach, using only one experimental curve for the model characterization, we are capable of accurately predicting the behavior of hyperelastic rubber-like materials under any loading condition.

In the present work, departing from the macromolecule behavior and integrating in the representative volume, we extend the multiscale modeling approach to reproduce the behavior of elastomers under isotropic and anisotropic damage using as reference one of the damage curves of the uniaxial, bi-axial, and pure shear tests.

For the damage curves of a material with isotropic behaviour, we obtain three parameters of the reference curve (Po, μ^*, λ) which allow us to model all the damage curves of the material by modifying only the parameter (λ) that represents the blockage associated with each polymeric chain in the material.

A Multicomponent Transeversely Isotropic Viscoelastic Model for Vascular Smooth Muscle Cells: The contribution of actin filaments and microtobules

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Vascular Smooth Muscle Cells (VSMCs) constitute the major cells in the media layer of the arterial walls. During biological processes, VSMCs adapt their structure, di mension, and shape in response to mechanical and biochemical stimuli, thereby maintain ing vascular tone to homeostatic levels [1]. The abnormal contractility of VSMCs is as sociated with the development of many diseases such as hypertension and aneurysms. Therefore, it has become a subject of significant interest to better understand the mechan ical behaviour of VSMCs in health and disease.

In the present study, we consider a finite element 3-Dimensional multiphase VSMC model, that encompasses the Nucleus and Cytoplasm surrounded by the Cell Membrane. The constitutive behaviour of each phase is described through a strain energy function. The VSCM intercellular space is a complex network comprising the actin and intermediate filaments that play a dominant role in the mechanical properties of cell [2]. Besides, it has also been reported that VSCM exhibits significant hysteresis phenomena when subjected to stretch and release cycles [3]. Based on that, we model the cytoplasm as a transversally isotropic viscoelastic material incorporating one fibre family. The nu

cleus is modelled as a visco-hyperelastic solid, whereas the cell membrane is modelled as a hyperelastic material.

To validate the predictions of our model, experimental data for various tensile tests, including uniaxial elongation, compression, and load/unload cycles, are used. The results of the simulation are in good agreement with the experimental studies. Further more, the model is utilized to investigate the effect of cytoskeletal structures on the me chanical behaviour of the cell. Our simulations indicate that the orientation and distribu tion of the filaments affect extensively the tensile properties of the cell.

This work is part of the Research Project "Multiscale modelling for the autoregulation of Microvessels, CARE" which was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the "1st Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment" (Project No. 876)

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Microstructure reconstruction using physics-aware multiscale VAE

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Microstructure reconstruction is a vital part of processing-structure-property-performance to understanding macroscopic properties and microstructure structure. The physical experimental method and numerical reconstruction method are the two main reconstruction methods. Since the former method is time and resource-consuming with a very limited size, while the latter is relatively time and cost-effective but suffers from a variable accuracy. With the development of deep learning in recent ten years, a different method has been utilized and become a keen direction. However, the explainability of such kind of methods are still unclear. The original Variational autoencoder(VAE) from encoding images to latent space Z and decoding the latent vector back to synthesize micrography. We encode the training images to several descriptors vector which makes the encoding process a supervised learning and decode back to micrography. Meanwhile, due to the limits of memory of GPU, the size of reconstructed images is limited with certain CNN parameters. We introduced a multiscale method which feed descriptors in different encoding layers and count descriptors in loss functions of different scale levels. By introducing descriptors into loss functions, we can understand how training data pairs are mapped and de-mapped. The new method is tested on a series of porous media microstructure images with distinct morphologies. Besides, various microstructural descriptors are used to quantify the discrepancies between the reconstructed and target microstructures.

Modeling plastic deformation and wear in contact problems by means of a multi-scale approach

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When modeling bodies in relative motion particular care needs to be devoted to describing the interaction between the surfaces, as this is essential to predict friction and wear. Ideally one should do that without making use of laws and parameters defined ad hoc by the user, which pre-determine the frictional response. To this end, atomistic simulations are well suited, as they make use of interatomic potential functions which can capture various material properties, including their adhesion, decohesion, and stacking fault energy. Provided the interatomic potential is well calibrated, friction and wear are emergent phenomena, so are dislocation nucleation and plastic behavior.

When one is interested in the tribological behavior of metal bodies with dimensions exceeding the nanoscale it would still be appropriate to have the same accuracy of atomistic simulations in describing contact sliding, at least when the loading is moderate, and the contact area is only a fraction of the nominal contact area owing to surface roughness. To maintain the advantages of atomistic simulations and tackle problems involving metal bodies at the microscale, we have designed a two-dimensional dual-scale method where the contact areas are described atomistically and the rest of the metal as a continuum deforming by means of dislocation dynamics [1].

This approach is similar to the modeling technique known as CADD [2], although it is better suited to solve contact problems, in that the deformation of the continuum domain occurs through a method based on Green's functions, where the dislocation image fields are just computed analytically in Fourier space [3].

The static equilibrium solution of the contact problem is obtained at each loading step through an iterative algorithm which relies on pad atoms linked to both domains to transmit forces and displacements.

The simulations compute the plastic deformation of the contacting bodies, by tracking the nucleation and glide of the dislocations, which are transmitted through the two concurrent domains. In the continuum the dislocations are represented by means of their linear elastic fields,

by means of which they interact with each other. The dual-scale simulations are validated against full-atomistic simulations for bodies at the nanoscale and used to model contact between bodies at the micro-scale.

Also, simulations are preformed to mimic the lubricating effect that can be provided by the presence of a lubricant or coating. While it is possible with our method to study any specific material system, provided the interatomic potential is available, we have here preferred to describe the effect of the lubricant or coating by means of a modified Morse potential, where the adhesive part of the function is tailored to vary attraction range and decay.

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On the Validation of Models for TRIP Steels with Bayesian-based Parameter Identification

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Transformation-Induced Plasticity (TRIP) alloys have been successfully employed in the automotive industry due to their remarkable combination of strength and ductility and reduced production costs. Their mechanical response stems from the complex interaction of crystallographic slip and mechanically-induced austenite-to-martensite phase transformations. Multi-scale models have been widely adopted to capture the macroscopic response of these materials using single-crystal constitutive models and computational homogenisation.

This work explores the validation of a recently-proposed model [1] for single-crystals undergoing martensitic transformation and dual-phase crystallographic slip. The generalisation of Patel and Cohen's energy-based criterion introduces the effect of mechanically-induced martensite transformations. A volume-preserving exponential mapping integrator for slip plasticity is coupled with a rate-dependent regularisation for plastic and transformation multipliers within a fully implicit return-mapping algorithm.

Using polycrystalline Representative Volume Elements (RVEs), the model's response is compared with macroscopic experimental data [2]. Bayesian optimisation is used to solve the inverse problem and find an appropriate set of constitutive parameters. Composite optimisation with quasi-Monte Carlo acquisitions and multi-fidelity Gaussian Processes are considered to speed up the calibration process. With the best-fitting constitutive parameters determined, the model's performance is assessed.

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Data-driven constitutive modeling with symbolic regression

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In this contribution we present a new procedure to automatically generate constitutive models of materials by using their experimental or artificially created stress-strain data. The procedure is based on symbolic regression which represents an evolutionary algorithm searching for a mathematical model in the form of an algebraic expression. This algebraic expression consists of a set of initially defined mathematical operations and functions. We illustrate an application of this algorithm by hyperelastic material models [1]. In this case, a strain energy function can be expressed in terms of the principal invariants of a strain tensor and calibrated in comparison to the above mentioned data. The expression of this function satisfying fitness and simplicity criteria is searched by the symbolic regression algorithm.

For the validation of the proposed approach, benchmark tests on the basis of the generalized Mooney-Rivlin model are presented. In all these tests, the proposed algorithm can find the predefined models. Additionally, this procedure is applied to the multi-axial loading data set of a vulcanized rubber. Finally, a data set for a temperature-dependent thermoplastic polyester elastomer is evaluated. In latter cases, good agreement with the experimental data is obtained.

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Multi-Scale Modelling and Characterization of Heterogenous Deformation in Austenitic Stainless Steel Welded Joints at Different Temperatures

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Heat-resistant austenitic stainless steels are widely used in the new generation of fossil fuel power stations due to their excellent high temperature behaviour. Similar austenitic stainless steel welded joints fabricated with gas tungsten welding are required when joining components, however they are known to suffer from premature high temperature failure. Observation of in-service failures revealed that cracks may nucleate either in the heat affected zone or in the weld metal. This work aims at identifying the local microstructural and stress-strain fields responsible for micro-cracks nucleation within the weld. To that purpose, a multi-scale micromechanics-based modelling framework which relies on representative weld microstructure models digitally reconstructed from EBSD measurements, and dislocation density-based crystal plasticity models to describe the behaviour of individual grains in each weld region. The single crystal models are formulated, calibrated and validated from a combination of uniaxial tests of welded specimens and representative volume elements of the polycrystals at the macroscale, and high resolution digital image correlation (HRDIC) techniques, micro-indentations and micropillar compression tests at the scale of individual grains. The predicted heterogeneous plastic deformation fields within the weld agree well with DIC-measured results at both 25ºC and 665ºC. Predictions of micropillar compression behaviour of individual weld single crystal phases are consistent with experimental data. The proposed methodology opens a new way for calibrating crystal plasticity material parameters through the use of HRDIC measured localised weld deformation and of digitally reconstructed weld microstructures.

Peridynamic Elastic Wave Propagation in Infinite 2D Domains: Designing Nonlocal Dirichlet-Type Absorbing Boundary

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In this presentation, we delve into the utilization of peridynamics (PD) for the propagation of elastic waves in unbounded domains. We focus on the development of absorbing boundary conditions (ABCs) derived from a semi-analytical solution of the PD governing equation in the exterior region. Our approach involves utilizing a finite series of plane waves, acting as fundamental solutions or modes, which align with the PD dispersion relations. These modes are carefully tailored to facilitate the transmission of energy from the interior to the exterior regions. To determine the unknown coefficients of the series, we employ a collocation procedure applied at subregions surrounding each absorbing point. The key information used in this process is the displacement field at a layer of points adjacent to the absorbing boundary. By leveraging this localized data, our proposed ABCs are able to eliminate the need for field variable derivatives and circumvent the requirement for Fourier and Laplace transforms, making them particularly suitable for PD simulations. Additionally, these ABCs seamlessly align with the numerical dispersion relations of the near field, ensuring a harmonious solution overall.

To assess the performance of our proposed ABCs, we present a series of examples that showcase their stability and accuracy levels. Even in scenarios involving highly-dispersive propagating waves, such as crack propagation in semi-unbounded brittle solids, our ABCs demonstrate remarkable efficacy. The results highlight the capability of our approach to accurately capture wave behavior while effectively absorbing outgoing waves at the boundaries of unbounded domains.

Overall, this research contributes to the advancement of peridynamic modeling in the context of elastic wave propagation. By constructing nonlocal Dirichlet-type absorbing boundary conditions, we enhance the realism and accuracy of PD simulations in unbounded two-dimensional domains.

Accelerated development of materials using high-throughput strategies and AI/ML[1]

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The dramatic acceleration of the materials innovation cycles is contingent on the development and implementation of high throughput strategies in both experimentation and physics-based simulations, and their seamless integration using the emergent AI/ML (artificial intelligence/machine learning) toolsets. This talk presents recent advances made in the presenter's research group, including: (i) a novel information gain-driven Bayesian ML framework that identifies the next best step in materials innovation (i.e., the next experiment and/or physics-based simulation to be performed) that maximizes the expected information gain towards a specified target (e.g., optimized combination of material properties, refinement of a material constitutive response), (ii) computationally efficient versatile microstructure image analyses and statistical quantification tools, (iii) formulation of reduced-order process-structure-property models that enable comprehensive inverse solutions needed in materials design (e.g., identifying specific compositions and/or process histories that will produce a desired combination of material properties), and (iv) high throughput experimental protocols for multi-resolution (spatial resolutions in the range of 50 nm to 500 microns) mechanical characterization of heterogeneous materials in small volumes (e.g., individual phase constituents in multiphase material samples, thin coatings or layers in a multilayered sample). These recent advances will be illustrated with multiple case studies.

Application of Physics-Informed Neural Networks for Multiphysics Problems and Nonlinear Constitutive Material Behavior in Solids

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Physics-informed neural networks (PINN) are a new tool for solving boundary value problems by defining loss functions of neural networks based on governing equations, boundary conditions, and initial conditions. Recently, it is shown that using first-order derivatives and combining equations from both strong and weak forms can lead to much better accuracy, especially when there is heterogeneity in the domain. This new approach is called the mixed formulation for PINN, which incorporate ideas from the mixed finite element method. In this method, the PDE is reformulated as a system of equations where the primary unknowns are the fluxes or gradients of the solution, and the secondary unknowns are the solution itself.

In this talk, we present results applying the mixed formulation to solve multi physical problems, specifically a stationary thermo-mechanically coupled system of equations. The focus is on two phase materials, where an inclusion is embedded within a matrix. We introduce a simple approach for parametric learning to address the limitations of PINN regarding computational cost and improves the network's ability to predict the response of the system for unseen cases.

Additionally, we applied PINN to solve the constitutive relations for nonlinear, path-dependent material behavior. As a result, the trained network not only satisfies all thermodynamic constraints but also instantly provides information about the current material state under any given loading scenario without requiring initial data.

Application of Physics-Informed Neural Networks for Multiphysics Problems and Nonlinear Constitutive Material Behavior in Solids

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Viscoelastic Drop Breakup in Cross Flow: A Numerical Study

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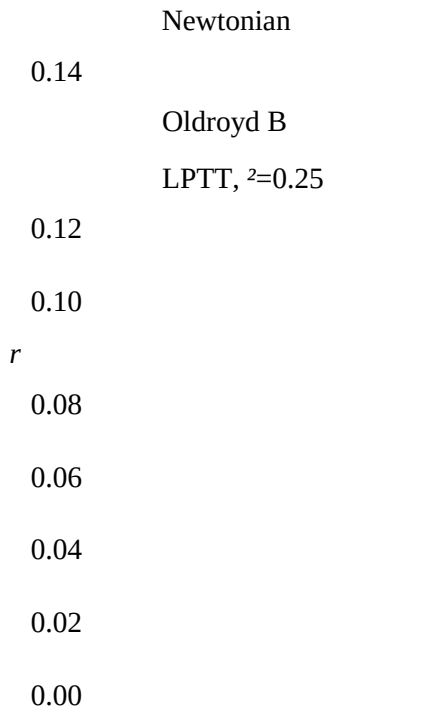
A drop subjected to high speed cross flow undergoes deformation due to aerodynamic force and breaks up into small droplets, also known as secondary atomization. Droplet breakup is observed in many natural and industrial processes such as rainfall, spray drying, inkjet printing, chemical reactions, combustors etc. The secondary atomization of Newtonian droplets has been extensively studied and detailed review is given by Guildenbecher et al. (2009). Jain et al. (2019) has explored the effect of density ratio and Reynolds numbers on the breakup of Newtonian droplets. Despite the prevalence of viscoelastic droplets in most of the industrial applications, limited literature exists on the secondary atomization of viscoelastic droplets.

The breakup dynamics of non-Newtonian droplets are significantly distinct from those of Newtonian droplets. Viscoelastic droplets have a propensity to resist breakup, and the daughter droplets produced upon breakup of viscoelastic droplets are larger in size than those produced from Newtonian droplets(Wilcox et al. (1961), Matta and Tytus (1982), Kumar Chandra et al. (2023)). The observed differences between viscoelastic drop breakup and Newtonian drop breakup are not yet well explained in the literature. This study attempts to understand the dynamics of secondary atomization of viscoelastic drops, which is affected by various physical quantities such as aerodynamic forces due to cross flow, shear rate-dependent viscosity of the drop and elastic and surface tension forces resisting drop deformation.

The Oldroyd-B and linear PTT which are standard constitutive relations for the viscoelastic fluids are considered for the study. The Oldroyd-B fluid accounts for the elasticity of the fluid, but it does not consider the shear rate-dependent viscosity. The linear PTT model, on the other hand, accounts for both elasticity and shear rate dependent viscosity of the fluid. Axisymmetric numerical simulations of drops in cross flow were conducted using the open-source solver Basilisk(http://basilisk.fr/src/). Basilisk utilizes the log-conformation tensor approach to solve the evolution equation of polymeric stress. Linear PTT relation has been implemented in the Basilisk solver.

Numerical simulations were conducted for a range of low to moderate Weber numbers and wide range of Deborah numbers. Oldroyd-B and linear PTT drops were observed to exhibit significantly different deformation characteristics from Newtonian drops. This study analyzes the observed differences between Newtonian, Oldroyd B and linear PTT fluids and explains the effect of elasticity and shear rate dependent viscosity on the droplet breakup dynamics.



Drop interface for non-dimensional times T = 0, 0.98, 1.31, 1.63, 1.96 at De = 10, We = 20, Re = 4000, density ratio is 150 and viscosity ratio is 100,

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A DG-FEM Method for Fluid-structure Interaction

Using Machine Learning Package

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Over past few decades, machine-learning methods have made great strides in both software implementation and hardware innovation. For software, there are many open sourced packages, such as PyTorch and TensorFlow. For hardware development, specialised chips for machine learning purposes have been manufactured, such as TPU from Google, IPU from GraphCore and AI processors from Cerebras. The combination of both provides powerful infrastructure for implementing machine learning algorithms such as neural networks.

These developments are driven by the optimisation of basic algebraic operations on different computing architecture at the low level. In this study, we intend to leverage these infrastructures to develop finite element method (FEM) for fluid-structure interaction problems, a multi-physics problem frequently occurred in many engineering applications. To maximise the parallelization capability of ML packages, we chose the high order discontinuous Galerkin FEM (DG-FEM), which is intrinsically suitable for parallel code. The method is implemented matrix-freely. The interaction between fluid and structure is solved in an arbitrary Lagrangian-Eulerian framework and discretised monolithically. The discretised system is solved by either multi-grid methods or a multi grid preconditioned GMRES solver. Under this high-order DG discretization, we explore the optimality of the *p*-multigrid method combined with algebraic multigrid (AMG). The coarse meshes used by AMG are generated by space-filling curve. We show that, in some cases, the number of multigrid cycles is independent of the problem size. The code is then verified by

convergence study on analytical solutions or manufactured solutions.

Unleashing Emergent Behavior: from Slime Molds to Swarm Robotics

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Soft materials have captivated engineers with their unique properties of low density, deformability, and customizability. However, conventional top-down engineering approaches struggle to achieve complex macroscale behavior. Drawing inspiration from the bottom-up paradigm of biological systems, we delve into the phenomenon of emergence through slime molds and fungi, which exhibit remarkable optimization capabilities. Through a theoretical and computational framework, we uncover the feedback between macroscopic features and local mechanical properties, leading to the coordinated emergence of network morphology. Tailoring the microstructural architecture and optimizing constituent materials allows us to realize custom properties in soft materials. To simulate slime molds in 3D space, we propose a phase-field scalar variable for network evolution and a diffusive-advective process for nutrient distribution. Overcoming challenges of coupled physics, high-order partial differential equations, and complex evolving geometry, our framework enables high-fidelity simulations. These simulations deepen our understanding of how slime mold networks grow, survive, and optimize nutrient redistribution for proliferation. Expanding our research, we leverage machine learning to transfer organization principles to swarms of kilobots, small ground drones. This integration of machine learning and swarm robotics enhances adaptiveness, enabling coordinated behavior with bio-inspired decentralized intelligence. Our interdisciplinary investigation advances the microstructural design of active soft matter, opening avenues for self-healing materials, sustainable building elements, and coordinated drone swarms. The impact of this research extends to fields such as soft robotics, tissue engineering, and medicine, where the manipulation of emergent behavior holds promise for transformative

applications.

On the modeling of particle cavitation in rubber-toughened amorphous polymers

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Key Words: Rubber-toughened amorphous polymers, Internal particle cavitation, Constitutive model, Finite element analysis, Parameter identification

Amorphous polymers have been widely used in aeronautics, automobile, structural and electronic applications due to their excellent thermal, optical, chemical and mechanical properties. Moreover, these materials can be easily tailored through suitable manufacturing processes at low production costs to fulfill specific applications. In particular, the addition of rubber particles improves their toughness, at the expense of losing some of the material's strength.

Rubber particles provide a transition from brittle to ductile fracture by promoting extensive plastic deformation that allows for the dissipation of large amounts of energy through either crazing or shear yielding. As a result, the prediction of their thermomechanical response is not straightforward and accurate constitutive models are currently lacking.

In the present contribution, a recently proposed finite strain visco-elastic visco plastic constitutive model [1] is extended to predict the nonlinear response of rubber toughened amorphous polymers. In this context, the nucleation, interaction and growth of voids are

accounted for. A nucleation law is established to predict cavitation under volumetric strains based on a well-established nucleation criterion [2]. A modified version of the well-known Gurson's potential is adopted to capture the void's growth, ensuring the coherence in the energy dissipation between the macro and microscales. A fully implicit integration algorithm is established, and a decoupled three-stage optimization-based calibration strategy is designed to identify the model's material parameters efficiently. The results highlight that the model can capture the typical behavior of amorphous polymers, as well as the decrease of stress associated with the increase of the void volume fraction.

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Investigation of Frictional Sliding Behavior of Rough Surfaces using Maxwell-slip Model

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Frictional sliding has been investigated in many fields, including aerospace industry, machining industry, wind energy industry, controlled mechanical systems, atomic friction, geomechanics and particularly tribology. It may cause a reduction in control system performance, larger settling times, vibration and noise, and wear and tear in engineering applications. In geomechanics, tribology, and atomic friction, frictional sliding is studied to comprehend the mechanisms that cause stick-slip or steady sliding behavior. This study aims to investigate the roughness effect on the dynamic behavior of frictional interfaces. We model a rough elastic body at the microlevel using the Maxwell slip model by introducing a randomness to the initial positions of the blocks of Maxwell slip model by using beta probability distribution function (PDF). Surfaces with various roughness values are imitated by changing the shape parameter of beta PDF. Sliding of the blocks on a rigid substrate occurs by a constant speed driver that is connected to all blocks by the springs carrying only tangential load. Coulomb friction law is assumed at the interface. Macroscopic frictional behaviors, i.e., stick-slip and steady sliding, are captured by this model that depicts a rough elastic surface at the microlevel. Our simulation results showed that rougher surfaces are prone to exhibit steady sliding behavior whereas smoother surfaces are prone to exhibit stick-slip behavior.

Multiscale modeling of graphite oxidation in water ingress accidents of high temperature gas-cooled reactors

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Water vapor ingress is one of the probable accidents in high temperature gas-cooled reactors (HTGRs), which can oxidize vulnerable graphite components and deteriorate integrity of fuel elements. However, it is unfeasible to conduct the graphite oxidation tests by mimicking the large-scale setup of the HTGR core system. In this case, numerical modeling of the graphite oxidation in water ingress accidents is an alternative method to predict and evaluate the global reaction behaviors in the core. The oxidation of the fuel elements occurs at two different scales and needs to be considered simultaneously in order to understand the oxidation behaviors during an accident. In this study, a multiscale modeling framework is established to investigate the oxidation behaviors of graphite in water vapor with coupled dual scale models. The macroscale model consists of a prismatic fuel block with a coolant channel to predict the water vapor permeation and location effects. The microscale model reconstructed using the X-ray computed tomography images estimates microstructure changes by oxidant flow. The oxidant concentration and temperature distributions obtained at macroscale are used as oxidation environments for the microscale analysis. The results are compared with experiments. The simulation results analyze effects of temperatures at the inlet and fuel on the distribution of water vapor in the graphite materials.

Experimental and micromechanical modelling studies of the precipitate size effect on the creep response of P91 martensitic steels

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High performance martensitic heat resistant steels are widely used in fossil fuel power plant industry due to their good creep resistance at high temperatures. In-depth understanding of the high temperature inelastic deformation mechanism of such steels is crucial to ensure the reliable, safe and efficient operation of the power plant. The purpose of this paper is to study the creep mechanisms with regard to the microstructure of the P91 martensitic steel at high temperature by means of experimental characterisation and finite element simulation[1].

In the present paper, apart from the standard heat treatment (holding at 1060 ◦C for 40 min and then at 760 ◦C for 2 h) for the as-received P91 steels, secondary tempering treatment has been applied with different tempering time periods, e.g., 0 h (T0), 10 h (T10) and 20 h (T20) at 780 ◦C. The effects of tempering duration on the creep response of the P91 steel at 600 ◦C and on the precipitate size were then experimentally examined. In order to quantify the effect with respect to the microstructure, crystal plasticity based micromechanical finite element model was developed based on the measured microstructure[2]. The crystallographic slip at the block level is accounted for using an exponential type of constitutive flow rule and the precipitate size effect is represented through the use of an internal variable in association with the slip resistance. The results

show that the secondary tempering duration can significantly affect the creep behavior of the martensitic steel. It is found that with increasing tempering time period the precipitate size increases, which could lead to detrimental effect on material's creep resistance. Furthermore, the FE model with exponential type of flow rule has capability to examine the microstructural effects on the creep behavior at a wide range of stress levels through the comparison with the experimental data. In addition, it shows that the accumulated equivalent plastic strain during the creep is strongly heterogeneous and the levels of the strain localization depend on the tempering duration.

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Modeling of High Strain Rate Effects on the Mechanical Behavior of Concrete Using Smooth Particle Hydrodynamics

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Compressive strength is a crucial mechanical property of concrete for structural applications, typically determined through quasi-static experimental testing. However, concrete may experience significantly higher strain rates during severe seismic events, resulting in varying stress states and failure patterns. Experimental techniques using hydraulic and drop weight impact testing machines, as well as split Hopkinson pressure bar devices, have been employed to study dynamic concrete behavior at strain rates ranging from $10^{-6}$to 10 s^{-1}[1-3]. Moreover, measuring forces or stresses at high strain rates can be challenging, particularly when fragmentation occurs [4]. In this research, Smooth Particle Hydrodynamics (SPH) is employed to investigate the dynamic compressive strength of concrete at high strain rates. The study focuses on the influence of strain rates on load-displacement curves, maximum compression strength, and the temporal evolution of failure patterns. To effectively tackle the plasticity phenomenon, RHT concrete model [5] is combined with the SPH numerical formulation. The RHT model incorporates concrete strength behavior through three different surfaces: elastic limit, failure, and residual resistance. Material parameters for the p-α equation of state and the strength model are adopted from the literature. The simulations are performed on a concrete cube subjected to uniaxial compression test at constant-speed load. The results show a nearly linear

increase in normalized maximum strength with increasing strain rates. Damage patterns are observed to concentrate at higher strain rates, with arc-shaped surfaces developing markedly in the specimen. Overall, this research provides insights into the dynamic compressive response of concrete under high strain rates, offering a comprehensive understanding of its mechanical behavior in such conditions.

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On the integration of domain knowledge and branching neural network for fatigue life prediction with small samples

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As one of the most common failure modes in engineering, fatigue is known to be susceptible to a variety of factors, e.g., material characteristics and loading patterns, with non-negligible uncertainties induced by defect sizes, component geometries, etc. Traditionally, fatigue failure is considered as an irreversible process of energy dissipation, associated with degradations in microstructural features and mechanical properties of materials. Along this line, numerous fatigue life models have been presented over the hundred years. However, due to the incomplete understanding of fatigue failure mechanisms, these models rely heavily on experimental observations and researchers' genius, which makes them essentially empiricism-based and short of reasonable accuracy for practical applications.

In recent years, machine learning has emerged as a promising tool for unraveling the complexities of fatigue failure processes, leading to a new trend in developing data-driven fatigue life models. In this context, artificial neural network (ANN)-based models have demonstrated their competence in achieving satisfactory prediction accuracy for complex fatigue issues. However, it is widely recognized that these models are easy to be afflicted by the insufficiency of training data in practice. Aimed to this drawback, we proposed a novel data-driven model integrating domain knowledge and ANN for fatigue life prediction with small samples. In the model, a subtractive clustering-based procedure of representative training data identification is implemented at first, and traditional fatigue life models are then employed to generate pseudo labels for data augmentation. To avoid the contamination of theoretical biases, we further devised a new ANN typology, called

Branching neural network for model training. Our proposed model was experimentally validated through three distinct cases studies.

Multi-scale effective elastic properties homogenization and finite element simulation of origami-inspired foldable structures

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Origami-inspired deployable folding structures have found increasing interest in space, civil architecture, robotics, flexible electronics, biomedical engineering, and biomimetic engineering. These deployable structures were traditionally made of metallic materials. In recent years, fiber reinforced polymers composites (FRPCs) have become increasingly popular in rigid and thin flexible regions because of their ability to achieve high packaging efficiency and lightweight jointless deployable structures manufactured through different methods. It is of high importance to optimize the folding structures using the computational tools for which the elastic constants are required. Because a large number of composites materials combinations are possible for which the experimental characterization is challenging. Therefore, a generic virtual characterization framework is needed to address this problem.

This work will describe a generic X-ray computed tomography (XCT) driven framework based on voxel modeling approach to virtually characterize the smallest building block of full-scale folding structures. Meso-scale real representative volume element (RVE) description is developed from the XCT images using the supervised segmentation method based on the parameters obtained from the structures tensor approach. Then, the micro-scale homogenization schemes are used in the determination of

the effective properties of each voxel using the fiber and matrix elastic stiffness properties. The meso-scale effective properties of the RVE are calculated employing the orientation averaging method.

Finally, the predicted elastic constants based on this generic XCT-driven framework are compared to the experiments to evaluate the efficacy of the proposed generic virtual characterization framework. Also, the finite element simulations of the folding structures are carried by using the predicted elastic stiffness properties and comparison is made to the fold experiment.

Multiscale modeling approaches for nonlinear porous thermoplastic polymers

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Some recent multiscale approaches are proposed for porous thermoplastic polymers where the material model of the matrix is either elasto-plastic or viscoelastic-viscoplastic.

A first approach deals with an elasto-plastic hardening, unreinforced or reinforced matrix phase. The cavities can be spheres, long or short cylinders. The approach is able to predict plasticity under hydrostatic loadings or any other stress triaxialities. It is based on the definition of an alternative microstructure made of elasto-plastic inhomogeneities embedded in a homogenized porous matrix phase, and the volume fractions are determined from a maximum packing argument. The effective properties of single hollow solids are computed with an energy-based approach coupled with full-field finite element (FE) analyses. Next, the alternative microstructures are homogenized with mean-field (MF) models. For reinforced porous materials, a two-level method is adopted, where the proposed approach is used at the lower level to obtain a fictitious homogenized matrix, in which reinforcements are embedded at the upper level. The present work is restricted to monotonic and proportional loadings and to the secant formulation of isotropic or transversely isotropic elasto-plasticity. However, no constitutive models are supposed or identified. The predictions were verified against reference full-field FE results on the actual microstructures in 3D and 2D plane strain or stress, for arbitrary stress triaxialities, and good agreement was found in all cases.

A second approach is proposed for porous thermoplastic polymers with coupled viscoelastic-viscoplastic behaviour. It is an incremental-secant method whiih relies on a fictitious unloading of the composite at the beginning of each time step. Then, a thermoelastic-like Linear Comparison Composite (LCC) is constructed from the computed

residual state directly in the time domain. The method provides naturally isotropic per-phase incremental- secant operators for isotropic VE-VP constituents. It takes into account both the first and the second statistical moment estimates of the equivalent stress micro-field. The formulation is able to handle non-monotonic, non-proportional and multi-axial loading histories. Its accuracy was assessed against full-field finite element (FE) results for different microstructures and loadings. Its computational cost is negligible compared to FE analyses while accuracy ranges from acceptable to excellent.

Finally, current work on data-driven and machine learning multiscaling approaches for nonlinear porous polymers is presented.

A Constitutive Formulation for Styrene-Based Shape Memory Polymers That Incorporates the Mullins Effect

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A styrene-based copolymer is a kind of thermally induced shape memory polymer (SMP) with a light weight and a high shape recovery ratio. This work will reveal that this type of SMP exhibits the so-called Mullins effect when deformed cyclically below the glass transition temperature (Tg). Such behaviour enables styrene-based SMPs to show a better shape recovery behaviour than other well-known SMPs due to the formation of super-molecular structures. The influence of the Mullins effect on the free recovery behavior of SMPs has not yet been addressed in the published literature.

In this work, a series of uniaxial cyclic tension tests in tension were conducted to identify the softening effect during the molecular chains' stretching process, as shown in the Figure, the resulting stress in the reloading part of each cycle falls below that of the initial cycle for the same applied strain, and an increasing strain amplitude results in a greater softening upon reloading, which is the so-called Mullins effect. A novel constitutive formulation for the styrene-based SMP that incorporates the Mullins effect in its cyclic behaviour is proposed based on the four-element network model first reported by Nguyen et al. (2008). The constitutive model is implemented numerically into the finite element method using an Euler Forward approach, and its calibration is carried out from dynamic mechanical analysis (DMA) and uniaxial tension tests at different temperatures and strain rates. The predictive capabilities of the model are independently verified through published data, and it reveals that styrene-based SMPs can exhibit a better free shape

recovery behavior under cyclic loading at temperatures below Tg than above. Experimental work is ongoing to identify the influence of Mullins effect on the free shape recovery of styrene-based SMPs.

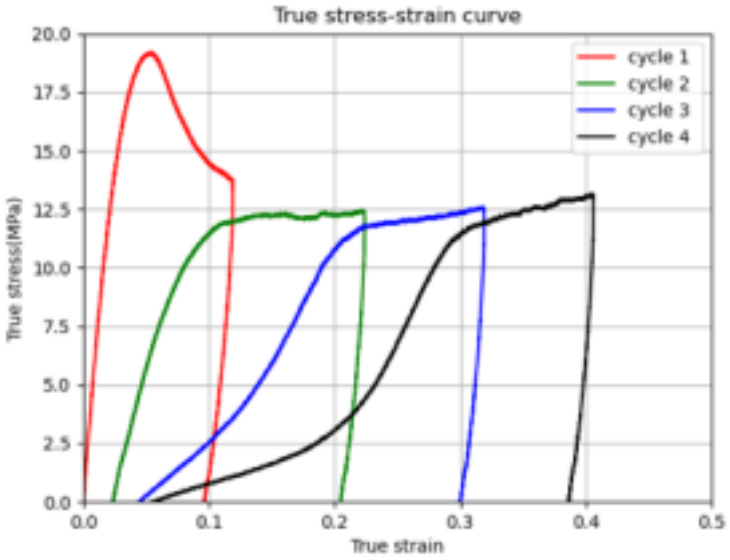

Figure True stress-strain responses from uniaxial cyclic tension test with increasing strain amplitudes

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Modular Supercomputing for High-Performance Simulation of Diblock Copolymer and Solvent Mixtures

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In this research, we describe the implementation of DCAT, a parallel, high-performance solver for the Uneyama-Doi (UD) model [1-3], dedicated to studying the multi-scale, multi-physics problem of diblock copolymer and solvent mixtures [4]. This solver is optimized to run on CPU-based systems, and leverages modular supercomputing techniques to couple with the particle-based code SOMA [5] which, on the other hand, uses the power of modern GPUs. The ParTec ParaStation MPI has been employed to run both codes as part of a heterogeneous MPI job.

The core of our implementation is a C++ code employing a semi-implicit Fourier spectral method, which permits the use of significantly larger time steps in comparison to explicit methods, while avoiding the need to solve complex systems of differential or algebraic equations. This reduction in computational overhead ensures faster simulations, enabling researchers to explore bigger parameter spaces in their investigations.

The FFTW library has been employed for FFT related calculations. Both shared and distributed memory parallelized versions of FFTW have been employed. This combination optimizes data exchange between nodes, enhancing overall performance and scalability. Additionally, we leverage the parallel HDF5 library for efficient I/O operations, enabling seamless handling of large-scale simulation data.

The UD model we adopt in our implementation provides a highly accurate representation of diblock copolymers' behavior, which finds widespread applications in diverse fields, including materials science, nanotechnology, and pharmaceuticals. Through

comprehensive performance evaluations, our research showcases the potential of modular supercomputing, for coupling of different types of solvers in addressing computationally demanding problems, especially in the realm of diblock copolymers.

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Comparison of Hemodynamic Characteristics of Localized Aortic Valve Calcifications under Uniform and Helical LVOT Flows

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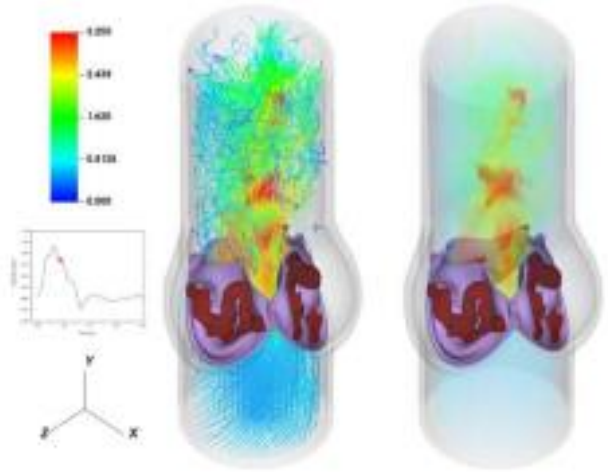
Blood rheology [1] has a critical role in both design process of patient-specific prosthetic heart valves, and identification and prediction of cardiovascular diseases. One of the most common valvular diseases is aortic stenosis (AS), which is caused by a reduction in the orifice area between the valve leaflets and leads to restriction of blood flow toward the body. Calcium build-up on leaflets plays a major role in the development of stenosis as calcium deposits increase the rigidity of the leaflets and hinder the functionality of the valve. Furthermore, the presence of non-uniform calcification patterns greatly affect the flow hemodynamics. AS can result in serious complications that may lead to mortality and morbidity in severe cases.

The motion and deformation of the localized calcified aortic valve leaflets as a result of coupled interaction between flexible tissue with calcium deposits and blood flow leads to a complex Fluid-Structure Interaction (FSI) problem. In order to create a realistic flow field around the aortic valve in terms of FSI modelling, it is crucial to define proper physiological boundary conditions, such as well-balanced LVOT (Left Ventricle Outflow Tract) flow rates accounting for AS based on corresponding calcification grades.

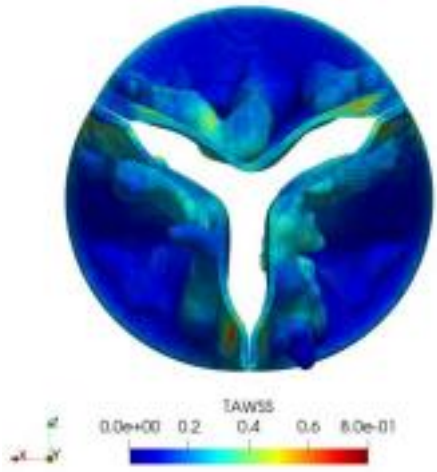
Although LVOT flow is almost uniform in most healthy cases, due to some LVOT disorders, LV (Left Ventricle) disfunctions, congenital anomalies and effect of AoSAs

(Aortoseptal Angles), it is observed that helical LVOT flow interacting with aortic valve leaflets leads to significant flow disturbances, unpresidential leaflet stress distributions and dynamics.

The aim of this study is to examine the effects of localized calcium formations for several grades on aortic valve leaflets under uniform and helical LVOT flow. To model the calcified aortic valve problem, we used IBFE (Immersed Boundary - Finite Element) method proposed by Griffith et al. [2]. FSI simulations of single-phase Newtonian blood flow under realistic boundary conditions are conducted, including helical inflow velocity profiles and an aortic outflow pressure represented by three-element Windkessel model. In order to quantify the critical parameters of blood flow and investigate the effect of calcification severity on the aortic valve functionality, numerous indexes based on transvalvular hemodynamics and Wall Shear Stress (WSS) are obtained. While energy loss, aortic jet velocity, kinetic energy and the average magnitude of the vorticity describe the transvalvular hemodynamics, WSS based indexes include TAWSS (Time averaged Wall Shear Stress), OSI (Oscillatory Shear Index), RRT (Relative Residence Time) and transWSS (Transverse Wall Shear Stress). Additionally, for the first time in the literature, the impact of right- and left-handed helical inflow from LVOT on aortic valve leaflets is analyzed and discussed with comprehensive indexes, including Helicity index and its intensity. Our initial results show a well-alignment with clinical observations (Figure 1).



a)



b)

Figure 1: a) Streamlines and volume contours of velocity magnitude [m/s], b) TAWSS [Pa] distribution on severely calcified aortic valve leaflets.

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Automatic Identification of Macroscopic Constitutive Parameters for Polycrystalline Materials based on Computaional Homogenisation

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A numerical framework for the automatic calibration of macroscopic constitutive parameters, based on the analysis of polycrystalline RVEs with computational homogenisation, is proposed. The said framework is composed of four building blocks: i) the RVEs of a polycrystalline material, and the crystal plasticity model in [1] to define the behaviour of each of grain, ii) the macroscopic von Mises elastoplastic model, along with the Nadai-Ludwik hardening law, whose parameters are calibrated, iii) the optimisation algorithms employed to solve the inverse identification problem, and iv) a first-order homogenisation approach to link the micro- and macro-scales.

Initially, the performance of several optimisation algorithms is assessed by means of a reference identification problem. Thereafter, different calibration strategies are tested, by employing distinct loading cases, definitions of the objective function, and evaluating the impact of the sequence of determination of the elastic and plastic parameters. The accuracy of the calibrated models is assessed by comparing the results of macroscopic simulations against an FE^2 model. The computing time of the FE^2 simulations is 5 orders of magnitude larger than that of the macroscopic simulations, demonstrating the suitability of this framework for obtaining efficient micro-mechanics-informed constitutive models. Finally, validation against experimental data [2] further establishes the robustness of the proposed approach.

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A Schwarz alternating collocation method for turbulent Rayleigh-Bénard

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A study of an alternating Schwarz domain decomposition method for a Rayleigh-Bénard problem is presented. The model equations are Navier-Stokes, continuity and heat equations in the case of infinite Prandtl number in a two-dimensional rectangular domain. The nonlinear evolution problem is dealt with an order two finite differences scheme in time and a collocation method in space. The stationary problem is solved with a Newton approach. Each step in the evolution problem or the Newton method is solved with a Schwarz domain decomposition technique. The domain is split into several subdomains with appropriate interface conditions. Their convergence properties are studied theoretically in a simplified domain divided in two subdomains. The convergence rate is less than one when an overlap is considered. The numerical resolution of the problem confirms the theoretical results. A benchmark with numerical solutions obtained with other methods validates the method. This methodology is parallelizable. Convergence is achieved for large spatial grids in both directions of the plane, and the turbulent regime can be addressed.

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Model order reduction for thermo-mechanically coupled multiphysics simulations including damage

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The analysis and prediction of damage onset and propagation within ductile materials under thermomechanical scenarios play an essential role in both research and industry. Many models in the literature concentrate solely on fracture and damage mechanisms while neglecting the influence of temperature. Therefore, simulations based on such models are often suitable only for some special cases that deviate far from true manufacturing conditions. On the other hand, multiphysics damage modeling considering temperature-dependent plastic flow is not only a challenging task but also usually leads also to computationally expensive simulations. This is mainly due to an increased number of degrees of freedom (in case of nonlocal damage) and the coupling between damage, plasticity, and temperature. Consequently, incorporating efficient model order reduction techniques into multiphysics models is an interesting and promising field of research, especially for industries focusing on real-time simulations.

The first objective of this work is to combine model order reduction approaches, such as Proper Orthogonal Decomposition (POD), with the gradient-extended damage plasticity formulation for finite strains by Brepols et al. [1] and to study its effect on

reducing computational costs. In the second step, POD is integrated into the thermo mechanically extended version of the aforementioned model (see Felder et al. [2]) to enable fast multiphysics damage-plasticity simulations. Finally, the new approach is investigated in several numerical benchmark tests to evaluate its advantages and disadvantages.

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Data-driven Derivation of Digital Twins from Conjugate, Multi-phase Food Processing Models

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A digital twin is a virtual set of information replicating its physical counterpart at the utmost fidelity. Digital and physical twin benefit from bi-directional data exchange that occurs in real time and over the whole process lifecycle. Until now, experts in the design phase have predominantly used simulation and data science technologies to explore what-if scenarios. In contrast to that, digital twins symbolize the endeavor to make simulation insights also available to the process that is in operation, such that it might make better-informed, autonomous decisions on its own [2].

The proposed computational framework enables the automated extraction of digital twins from existing simulation models in commercial software. Hence, it is designed to be readily applicable within the industry. Its usage is demonstrated with the derivation of digital twins that enable autonomous thermal food processing [1]. A software suite called TwinLab was developed to automate simulation model handling, training data selection, reduced-order model derivation and digital-twin-based control techniques in one framework.

Requiring the utmost accuracy of digital twins entails the setup of sophisticated, multi-physical simulation models to form an appropriate data foundation. To capture the product-process interrelationship better than with transfer-coefficient-based models numerously found in literature, a novel approach couples porous media food processing models with the non-isothermal flow and thermal radiation within a convection oven. Heat

and mass transfer and phase change effects of the food model are implemented in a conjugate manner. Comparing a conjugate simulation of a food item with a constant-heat-transfer-coefficient-based simulation reveals pronounced differences: The temperature locally differs up to E_{max} = 48 K (30.6% relative error). The water saturations differ with E_{rel} = 60%.

Providing real-time replication reveals that Digital Twins must solve much faster than a simulation model. This work demonstrates how digital twins can be trained with only one-to-two training data sets extracted from multi-physical simulation models. A proposed efficient design of experiment provides decision-support to select training data that ensure low test error of the twin on representative test data. In particular, root-mean-square errors for the best twins are 0.30–0.83 K. The time series' relative error of 0.18–0.49 % is superior to the validation errors of the employed food processing models. Attainable speed-ups of the digital twin compared to real time are approximately Sp ≈ 3.6 × 10^4, with characteristic solution times of one-tenth of a second – without imposing a noticeable computational cost on a single-core processor. Field data with 4649 points in space and one hour of real-time processing outputs can be predicted within less than half a second.

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DFT investigation of the structure, elastic and optical properties of mineral qatranaite.

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The compound $CaZn_2(OH)_6 \cdot 2H_2O$ was known in synthetic form for decades; recently, it was discovered in nature as a mineral qatranaite [1]. Its structure consists of vertex-connected Ca-centered octahedra and Zn-centered tetrahedra; the oxygen atoms at the vertices belong to hydroxyl or crystallization water; the whole structure is hold together by covalent and hydrogen bonds. Such construction may be considered prototypical for many complex oxides (or even beyond this class), combining general robustness with variability in chemical substitution or structural coordination.

We report an examination of the structure, electronic and optical properties of qatranaite utilizing density functional theory-(DFT-) based calculations. Furthermore, the elastic constants C_{ij} of qatranaite were calculated, using the stress–strain method. Based on the obtained data, the bulk modulus B, shear modulus G, Young's modulus E, Poisson's ratio, and elastic anisotropy A were also estimated.

Another interesting topic is the vibrational properties of qatranaite. We found that both Raman experimental data and our DFT results indicate that the wavenumber of vibrations involving Ca, Zn, and (mainly) O are situated below 600 cm^{-1}, whereas the those involving hydrogen (all of them having a small participation of oxygen) are spread over $700 - 3500$ cm^{-1}. The results of our calculations showed the four possible candidates for the bending

mode of a free water molecule: 103 (1643 cm−1), 104 (1655 cm−1), 105 (1661 cm−1), and 106 (1662 cm−1), which agrees well with other experimental work [2].

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Computational Homogenisation of CNT Reinforced Nanocomposite Undergoing Large Deformation Considering Different Periodic Boundary Conditions

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Elastomer nanocomposites reinforced by Carbon nanotubes (CNTs) are one of the promising candidates for advanced structural applications in various fields owing to their extraordinary properties. In this study, the elastic behaviour of such composite materials is investigated using a nonlinear finite element modelling (FEM) approach. The FE code is written in the C++ program language and builds on the deal.II library to analyse the large deformation of compressible and incompressible elastomer nanocomposites. To this end, a representative volume element (RVE) is modelled by dispersing several CNTs with random positions and orientations into the polymer matrix with different volume fractions. Two different approaches in the distribution of CNTs are investigated. In the first, the whole part of every nanotube is embedded inside the matrix without cutting the boundaries. In the second approach nanotubes can cut a boundary face and the reminder of the nanotube enters the matrix from the opposite boundary face making a periodic connected pattern. Both approaches are widely used in literature and produce repetitive RVEs. The first approach has the benefits of allowing for easier modelling and meshing while the second approach is assumed to produce more realistic microstructures; however, it presents meshing challenges as matched nodes are needed on opposite faces to apply admissible boundary conditions.

Moreover, various types of admissible boundary conditions including the so-called prescribed linear displacement, weak constraint constant tractions and periodic displacement with antiperiodic tractions are examined. Choosing a proper type of CNT

distribution pattern along with imposing proper boundary conditions to model RVEs under large deformation considering the accuracy, efficiency and convenience of the simulation is a key challenge addressed here. These different approaches are discussed, and the outcomes compared to experimental data to assess the various approaches.

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Multiphase flow coupled modelling in deformable dual-porosity media: theoretical derivation and numerical case

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Modelling of multiphase flow in deformable dual porosity media has attracted attention in the past decades, however, the effective stress equation and constitutive model development remain a challenge due to lacking a unified theory foundation. Moreover, the fluids in the void can either be studied separately or as an effective mixture fluid, the two views can lead to significant differences in both the thermodynamical framework and the multi-physics coupled equations.

This talk will describe the theoretical derivation and numerical case for the multiphase flow coupling in deformable dual-porosity media. Helmholtz free energy density has been used to establish the relationship between solids and fluids. The interaction of fluids in pore space and fracture space has been fully considered, leading to a new form of effective stress. The coupling of the large deformation of the solids and multiphase transport has been established leading to two general new constitutive models, one is based on treating the multi-fluids separately and another is on the effective mixture fluid view. The new mathematical equation for effective stress provides a most comprehensive model with the least assumption compared with existing models. Then the model was validated and applied to a real shale gas site for the prediction of fluid flow back and gas production.

This model may benefit the theoretical multi-physics research of fluid flow and the practical problem in geo-energy engineering such as shale gas or carbon capture and

storage.

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Physics informed neural network for solution of multispecies contaminant transport with variable parameters

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Multispecies pollutant migration is a natural phenomenon that frequently occurs in polluted groundwater systems [1]. Modeling the migration of pollutants in multispecies problems with variable transport parameters poses a significant challenge. Currently, most solutions for multispecies problems focus on constant parameters that affect the concentration distribution, rather than accounting for variable transport parameters due to the complexity of the modelled equation [2]. Deep neural network has gained considerable attention for its ability to handle strong nonlinearity in solving pollutant migration, but it has not been applied to multispecies problems with variable parameters.

In this paper, a physics-informed neural network (PINN) [3][4] that incorporates Resnet blocks [5] to solve multiscale multispecies pollutant transport problems is proposed. We analyze the effects of spatio-temporally varying hydrodynamic dispersion coefficients and transport velocity terms on the porous structure. The proposed model solves the pollutant transport problem by integrating multi-species partial differential equations into the loss function of a deep neural network. A typical PINN framework for solving this problem is shown in Figure 1.

Additionally, we introduce a new adaptive collocation [6] scheme that progressively

resamples and assigns more collocation points to regions with large model errors, based on a probability density function proportional to the residuals of the partial differential equation. We analyze the system for both steady and unsteady groundwater flow, as well as transient transport systems [2] and good results are obtained as shown in Figure 2. Compared to the original physics-informed neural network, the developed algorithms reduce errors by an order of magnitude and significantly improve its accuracy.

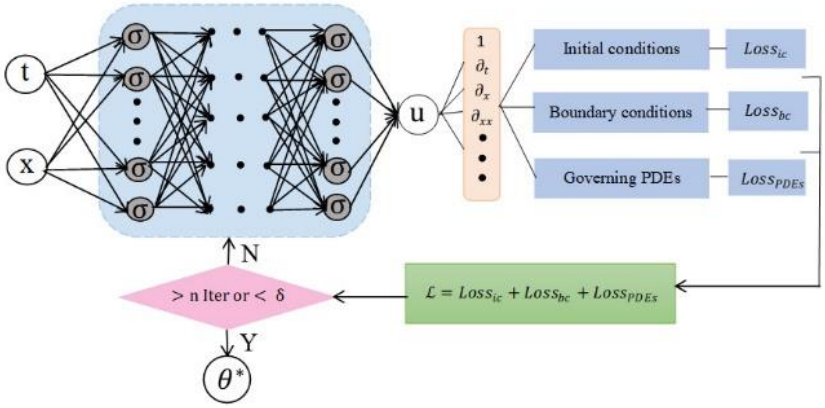
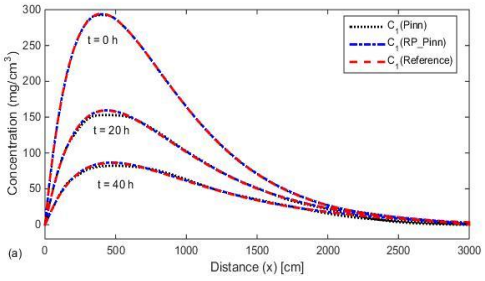


Figure 1 A typical PINN framework to solve the forward problem of nonlinear PDE.



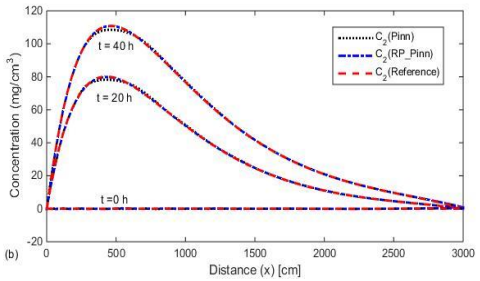


Figure 2 Concentration vs Distance for both species for steady transport in steady groundwater flow. The numerical results obtained by original PINN, RP-PINN, and reference solution have been compared.

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Physics-informed neural network for diffusion wave problem

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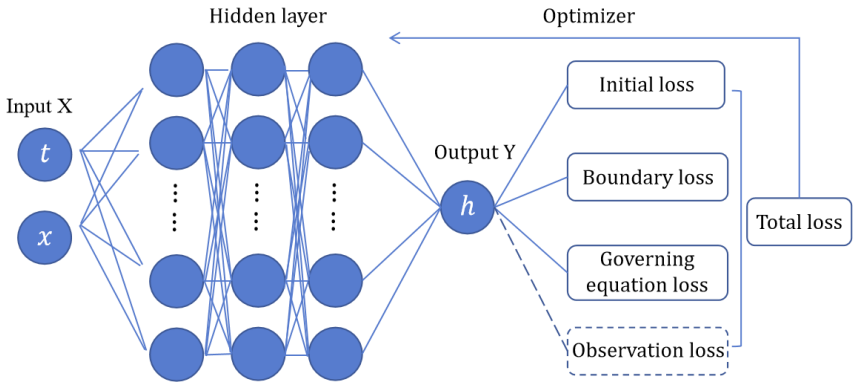
As an important nonlinear second-order simplified form of shallow water equation, diffusion wave model (DWM) has been widely used to deal with many problems, including simulating wave motion, urban waterlogging, dam-break problem[1]. Moreover, these problems can be coupled with other problems, for example, coupling with the convection diffusion equation can simulate the transport of pollutants. So, it is an important model in hydrology and hydraulics and there are numerous literature studies on solving diffusion wave equations using several numerical methods, including finite volume method (FVM), finite difference method (FDM), characteristics method.

With the development of computing power and deep neural networks, physics-informed neural network (PINN) has recently been used to solve ordinary and partial differential equations for both forward and inverse problems[2]. The PINN combines the prior physical knowledge with the data-driven structure of deep neural network, which is trained to approximate the solution of the problem as supervised learning. The advantage of PINN is twofold. First, it entails automatic differential technology, which can easily implement the training process, approximate the derivatives of the solution, and get the continuous solution in the whole solution domain. Second, the same framework can be used to solve both forward and inverse problems, and its implementation is straightforward and easy. The calculation process of PINN on the DWM is shown below.



This talk will describe the work on applying and improving PINN to solve the diffusion wave model in both forward and inverse problems. The improvement of the algorithm consists of the following three parts. In order to solve the gradient explosion in the training process caused by the characteristics of the diffusion wave model, the stop-gradient technique is adopted to train the neural network. To improve the effect of simulation and parameters prediction of PINN, the idea of time division and a new network structure are proposed. The latter two improvements are called TPINN and MPINN, respectively.

Seven examples are presented to verify the effectiveness of PINN and its improved algorithm on the diffusion wave model. The PINN solutions for forward problems are compared with the results obtained by some classical numerical methods, including fourth-order Runge-Kutta method, MacCormark method, while rainfall pattern is learned for inverse problem. TPINN is suitable for unsteady-state situations. When the rainfall pattern in the diffusion wave model changes with time, the error of the governing equation is easy to accumulate in the time direction. TPINN divides the time periods and reduces the error in each time period as much as possible to improve the error accumulation. MPINN changes the original fully connected network structure into a network structure composed of a family of activation functions, which is more complex and can represent a richer set of functions. The inverse problem is to learn the unknown rainfall rate in diffusion wave equation using the information of the observation. The learning effect of reducing the number of selected points in time and space is considered respectively and the learning error can be

controlled between 3%-10%. In practice, the selection points of increasing spatial position is much more complicated than that in time, and the selection of space points here can meet the actual engineering requirements. PINN, TPINN, MPINN can learn the rainfall pattern correctly.

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Modeling of partially oriented spring-exchange magnetic composites

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Hard magnetic materials are very important in modern technologies including automotive industry, energetics as well as different kind of sensors and actuators. Perfect permanent magnets should have high magnetic remanence, high coercive field and high value of the so-called energy product $|BH|_{max}$ (related to the energy of magnetic field outside a sample). In the family of hard magnetic materials a special meaning have those containing rare earth (RE) as well as transition metals. Unfortunately, resources of the rare earths are restricted, and therefore, findings of new hard magnetic materials without or with reduced RE content are of great importance. One of possible research directions is related to a possibility of coupling magnetically hard (HM) and soft (SM) phases in the so-called spring-exchange magnets where the hard part is a source of magnetic anisotropy and the soft phase should increase magnetic remanence. Surprising is relatively low progress in such composites [1]. One can observe that either the SM phase dominants for contributions of 20-30 % or a price of the composite is economically unacceptable. Therefore, the motivation of the present work is to theoretical study of the spring-exchange system including the most important parameters affecting magnetic characteristics.

The presentation refers to simulations of magnetization processes of the spring-exchange magnetic composites containing magnetically soft and ultra-high coercive phases. The unique approach is to include into consideration random orientation of magnetic anisotropy of the HM grains, which is close to real powders composites. In order

to modeling hysteresis loops a special disorder-based Monte Carlo procedure, suitable for irregular geometry of the composites, was applied [2]. The chosen system parameters were defined in order to modeling NdFe2B/Fe, FeCo/Fe and MnBi/Fe composites [1] The obtained results indicate a possibility to optimization of hard magnetic properties of the tested systems, regarding either enhancement of the $|BH|_{max}$ parameter or decrease of the hard magnetic phase content. The key meaning parameters are i) strength of magnetic coupling between the phases, ii) magnetic coercivity of the HM phase, iii) degree of the HM grans orientation and iv) composition. The presented results indicate possible research directions accounting different application requirements and an economic meaning, which is discussed in details.

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Thermodynamic equilibrium of large scale Monte Carlo magnetic simulations

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The presentation refers to Monte Carlo magnetic simulations and finite element scaling rules, allowing simulating magnetic mesoscopic systems [1]. The idea is to define a "super cell" (SC) consisting of many system nodes that are attributed to one node of the new enlarged system. The scaling rules consist in a redefinition of system Hamiltonian as a function of a scaling factor (size of the SC), including spin values and exchange integral parameters. Recently, we reported that in the frame of this procedure it is possible to simulate magnetisation processes of relatively large systems, including magnetic dipolar interactions, which is the main factor of computation power consumtion. Unfortunately, this approach leads to a disturbance of the thermodynamic balance expressed by acceptance probability in the Monte Carlo steps.

As a solution of this problem, we propose to provide the MC simulation simultaneously for the "super cell" and the enlarged system. Next, selected parameters are determined from the behavior of the SC and they are apply for the nodes of the enlarged system. This approach allows keeping the thermodynamic balance which is shown and discuses in details.

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Tritium transport in multi-physics modelling of large scale components for nuclear fusion using the MOOSE finite element framework

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Studies of tritium retention and permeation in the plasma-facing components of a fusion device are considered important for managing radiological risks and fuel inventory. Accurately modelling this, however, depends on coupled multiphysics at multiple length and time scales where large uncertainties remain in material properties, particularly as experimental data for the challenging fusion environment is not yet available. Calculations may need to take account of coupled neutronics, heat-transfer, and material damage, and span from molecular scale interactions between hydrogen atoms and metal-lattice defects at microsecond timescales to metre-scale, multi-material simulations over the many years of a component's lifetime.

We present the work to date to develop simulation capability for large, component-scale calculations of tritium transport in fusion devices using the MOOSE (Multiphysics Object-Oriented Simulation Environment) finite element framework. MOOSE is an open-source integrated modelling framework with proven scalability to tens of thousands of cores. This allows us to couple any combination of different physics modules, both pre-packaged and those we develop in-house, and deploy efficiently at ever-increasing scale and complexity on HPC resources.

Included in this work are uncertainty quantification tools, surrogate modelling, and Bayesian inference for exploring input uncertainties; coupling to material damage models

from the atomic scale; and exploring multiphysics couplings in large components such as breeder blanket modules.

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Investigating and predicting the permeability of porous media under compression

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The microscopic investigation of the stress/strain relationship in porous media is challenging due to its complex pore structure. Traditionally, researchers simplify the heterogeneous material using weak parameters. However, at the pore scale, the complex pore structure cannot be ignored, particularly when studying fluid behavior and transport properties within porous media. To investigate permeability and relative permeability of porous media under varying pressures, many researchers establish Finite Element (FE) models based on CT-micro-images for the simulation of solid phase, coupled with the Finite Element-Volume Method for the fluid phase. However, the FE method has inherent limitations in treating contact problems when the pore structure is closed under pressure, and the complex geometry of pore-scale porous material makes creating finite element meshes difficult. A specific tool is usually required to detect the surface information from the original CT image and create nodes and surfaces for the FE mesh accurately. Working with a large number of irregular meshes can induce long simulation times and high costs.

This paper presents a framework that uses the Discrete Element Method (DEM) to construct complex real shape models based on micro-CT images, which has advantages in contact problems. Three parameters were introduced to control the quality of the reconstructed models. The paper also analyses the effects of different parameter combinations. To validate the deformation result of the DEM simulation, the effects of these parameter combinations were analyzed using Finite Element Method (FEM) simulations.

After the method was established, the permeabilities under different pressure(strain) were simulated as data pairs, based on which a deep learning method has

been trained. The trained neural network shows a potential to predict permeability under different pressure(strain), while using the digital rock samples as input.

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The dramatic acceleration of the materials innovation cycles is contingent on the development and implementation of high throughput strategies in both experimentation and physics-based simulations, and their seamless integration using the emergent AI/ML (artificial intelligence/machine learning) toolsets. This talk presents recent advances made in the presenter's research group, including: (i) a novel information gain-driven Bayesian ML framework that identifies the next best step in materials innovation (i.e., the next experiment and/or physics-based simulation to be performed) that maximizes the expected information gain towards a specified target (e.g., optimized combination of material properties, refinement of a material constitutive response), (ii) computationally efficient versatile microstructure image analyses and statistical quantification tools, (iii) formulation of reduced-order process-structure-property models that enable comprehensive inverse solutions needed in materials design (e.g., identifying specific compositions and/or process histories that will produce a desired combination of material properties), and (iv) high throughput experimental protocols for multi-resolution (spatial resolutions in the range of 50 nm to 500 microns) mechanical characterization of heterogeneous materials in small volumes (e.g., individual phase constituents in multiphase material samples, thin coatings or layers in a multilayered sample). These recent advances will be illustrated with multiple case studies.

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Modelling the Impact of Insufficient Base Cleaning on Fresh Concrete Flow within Bored Piles using CFD

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The process of constructing bored piles is generally split into two stages: the drilling phase (demolition – removal – stabilization – cleaning) and the construction phase (reinforcement cage placement – casting – curing). During the drilling phase, loose sediment and debris from the ground surrounding the borehole becomes mixed with the support fluid – eventually settling on the base of the pile. Depending on the geology of the construction area, this debris will be comprised of some ratio of rock, clay, sand, soil and water. Prior to the construction phase, a cleaning bucket is used to remove this layer of debris at the base from the pile. However, the reality is there will always be some amount of debris on the pile base since the cleaning process isn't 100% effective. It is believed that this debris layer can have a negative impact on the quality of the final pile – leading to defects such as shadowing, inclusions and pour adhesion between concrete and the rebar cage.

The aim of this study is to investigate the impact of pile base debris on the overall flow of fresh concrete and conclude whether it can be linked as a root cause to certain observed defects within the industry. A pure CFD (Computational Fluid Dynamics) approach has been taken, and the multiphase solver multiphaseInterFoam within OpenFOAM has been utilised to model this process and capture the flow interactions between support fluid, concrete and debris. Parameters such as debris rheology, debris layer thickness, concrete rheology and concrete inlet velocity have been investigated using a high-fidelity 3D pile geometry with explicit modelling of the rebar cage.

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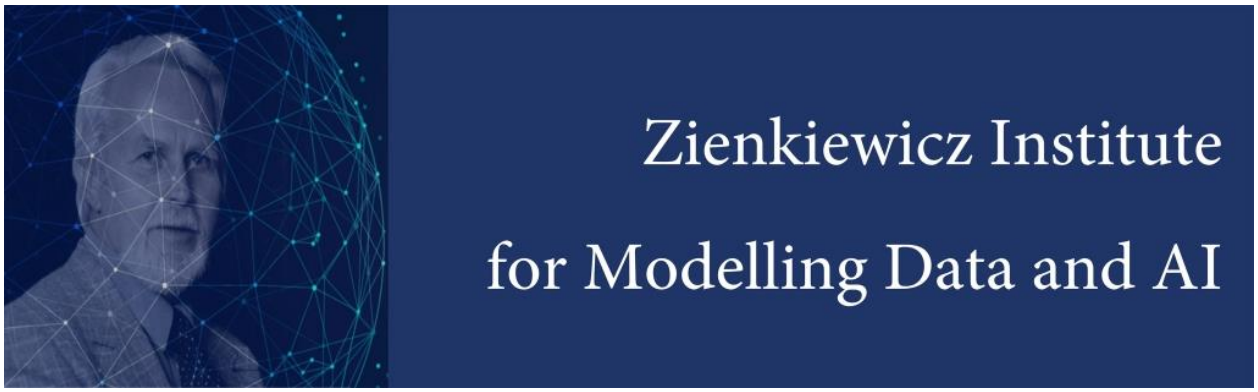

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Solving Adhesive Contact Problems based on a Primal-Dual Active Set Strategy

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Over the years, substantial research has focused on understanding and modeling of bonding and cohesive behaviors. However, there is a noticeable lack of approaches that explore the interplay between normal and tangential adhesion with friction in the existing literature. Typically, these aspects are treated separately, which hinders a comprehensive understanding of adhesive interactions.

The model proposed by Rauos, Cangémi and Cocu [RCC] stands out as one of the most promising approaches for such modelling adhesion coupled with friction [1]. This model follows Fremond's concept of adhesion which tackles the problem from a phenomenological standpoint, it treats adhesion as a single variable, varying from full adhesion to complete separation. The resulting interface model comprises a double set of contact constraints and an equation governing the evolution of adhesion intensity over time.

This work presents an implementation of the RCC model in a large strain finite element

framework, using a mortar contact discretization method. Adhesion contact conditions are enforced as nodal constraints. A primal-dual active set strategy is used to incorporate the active set search process directly into the semi-smooth Newton method, resulting in an efficient and robust solution scheme [2]. Non-linear complementary functions are rewritten to include adhesive interactions at the interface, based on previous works. The approach is validated using numerical examples that highlight different contact scenarios with different adhesive regimes operating at the same time.

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Dislocation-based finite element method for homogenized limit domain characterization of porous media and structured metamaterials.

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Keywords: Limit Analysis, Optimization Program, Linearized Domain.

Heterogeneous, porous, and micro-structured materials have been the object of multiscale and homogenization techniques aimed to recognize the elastic properties of the equivalent continuum. The proposed investigation delas with the mechanical characterization of the heterogeneous material through analyzing the ultimate strength using the limit analysis of the Representative Volume Element. To get the desired material strength a novel Finite Element formulation based on the derivation of self-equilibrated solutions through the finite elements devoted to calculating the lower bound theorem has been implemented together with the limit analysis in Melàn's formulation. The finite element formulation is based on discrete mapping of Volterra dislocations in the structure using isoparametric representation. Using standard finite element techniques, the linear operator V, which relates the self-equilibrated internal solicitation to displacement-like nodal parameters, has been built through finite element discretization of displacement and strain. The numerical formulation used a linearization of the limit domain in the component of stress that originates from the Schleicher-Mises limit domain with different resistance of the material in tension and compression. The underestimate of the material response depending on the linearization has been corrected using the penalty factor described synthetically in the figure. The results have furnished the limit stress at several elementary loads simulating uniform stress states of the homogenized element. The limit domain of the homogenized

material has been obtained through its intercepts with the axes of the stress space. The obtained strength allows to formulate both the linearized and the nonlinear limit locus of the homogenized material hence furnishes the starting point for further limit analysis of the structures whose elementary volume has been described through the proposed approach.

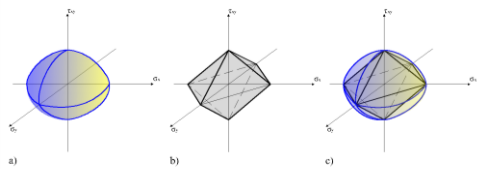

Figure 3 Non linear (a) and linear (b) domain and their superimposition (c)

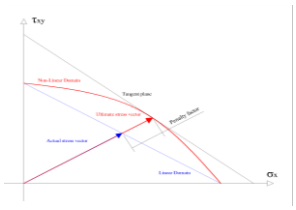

Figure 4 Penalty factor on actual stress

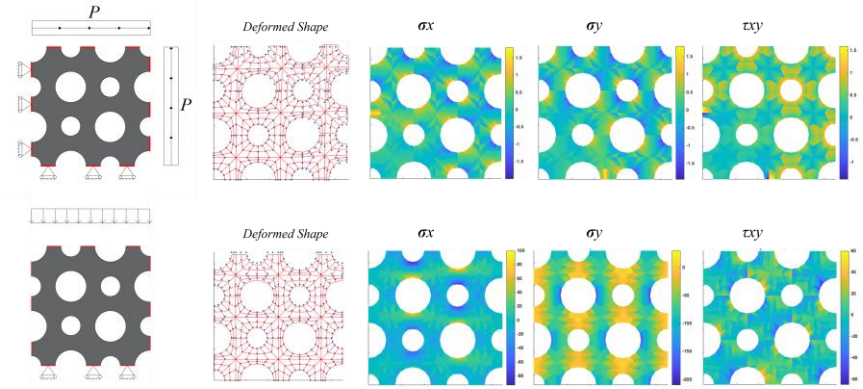

Figure 5 Porous RVE VFEM solution

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