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Computational Modeling of Complex Materials Across the Scales

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May 13-16, 2025 - Gustave Eiffel University, Champs-sur-Marne, France

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Physics-based Machine Learning for Computational Failure Mechanics

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Keywords: ϕML, Phase-field approach, brittle and ductile solids, Fracture and Fatigue

Abstract. This study introduces a physics-based machine learning (ϕML) framework for modeling both brittle and ductile failures. Unlike physics-informed neural networks, which solve partial differential equations by embedding physical laws as soft constraints in loss functions and enforcing boundary conditions via collocation points, our framework integrates physical principles, such as the governing equations and constraints, directly into the neural network architecture. This approach eliminates the dependency on problem-specific retraining for new boundary value problems, ensuring adaptability and consistency. By embedding constitutive behavior into the network's foundational design, our method represents a significant step toward unifying material modeling with machine learning for computational fatigue and fracture mechanics. Building on this foundation, synthetic datasets generated from finite element-based phase-field simulations are employed to train the proposed framework, focusing on capturing the homogeneous responses of brittle and ductile fracture/fatigue. Detailed analyses are performed on the stored elastic energy and the dissipated work due to plasticity and fracture, demonstrating the capability of the framework to predict essential fracture features.

The proposed ϕML framework overcomes the shortcomings of classical machine learning models, which rely heavily on large datasets (data-hungry) and lack guarantees of physical principles. By leveraging its physics-integrated design, the ϕML framework demonstrates exceptional performance in predicting key properties of brittle and ductile failures with limited training data.

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MODELING OF SHORT CRACK PROPAGATION: COUPLING PHASE FIELD METHOD WITH DISCRETE DISLOCATION DYNAMICS

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Key words: Fracture, Phase field, Dislocation dynamics

Abstract.

The propagation of short cracks in FCC metals is strongly influenced by microstructures, associated with the linear defects of the crystals, i.e., dislocations.
In this work, a new coupling between two methods at the mesoscale is proposed to investigate the interaction of moving cracks with three-dimensional dislocation microstructures. First, crack propagation is predicted by a phase field model [1]. In this approach, cracks are described by some continuous damage field that evolves to minimize the total free energy, including stored elastic energy and surface energy associated with the crack. Second, dislocation microstructures are handled by a Discrete Dislocation Dynamics (DDD) model that describes plastic deformation by the movement of dislocations under external loading.

To couple both models, the DCM (Discrete-Continuous Model) [2] approach is used, where dislocations are described by continuous fields (eigenstrain or Nye tensor) in an elastic solver. Fast Fourier Transform (FFT) based solvers are used for their computational efficiency. Particular discretization schemes have been adopted to minimize the smoothing of dislocation cores, usually performed in DCM approaches. The different schemes are carefully analyzed with respect to the quality of the predicted fields. In addition, the resulting model is implemented using efficient parallelization solutions.

Thanks to this new coupling, we have been able to study the elastic shielding on crack propagation according to the nature of the slip systems and the dislocations density. We have also been able to investigate phenomena and ingredients rarely accounted for, such as dislocation cross slips close to the crack front or the influence of the number of sources. This mesoscale method constitutes a breakthrough for the thorough analysis of physical mechanisms controlling the early stages of fracture in metallic materials.

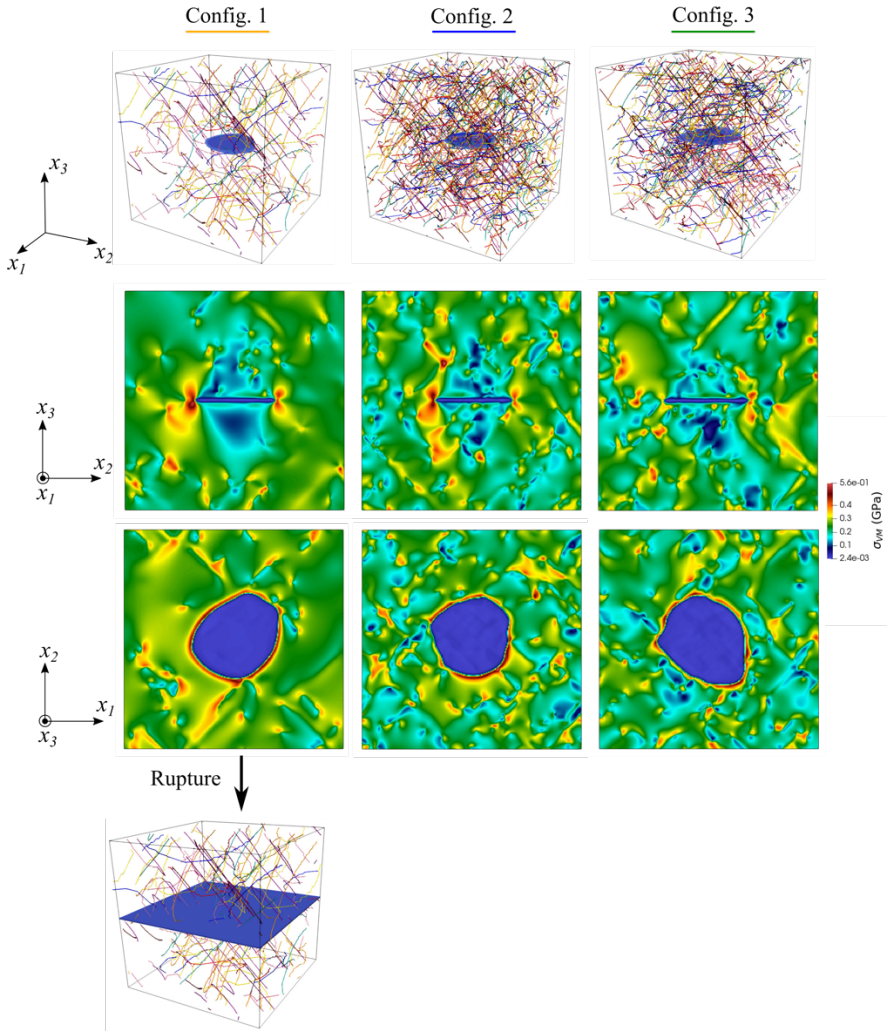

Figure 1: Mode I cracks with increasing initial dislocation densities from left to right. Top: crack and dislocations microstructure; middle: Von Mises equivalent stress field (side and top views).

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DEFORMATION DEPENDENT CONDUCTIVITIES IN A POROUS ELECTROMECHANICAL SYSTEM FROM VARIATIONALLY CONSISTENT HOMOGENIZATION

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Key words: variationally consistent homogenization, effective conductivities, large deformations

Abstract. Electrolysis cells represent an important application of porous electromechanical modeling, as they constitute a substancial green technology for future energy transformation. These cells are composed of a catalyst coated membrane (CCM), which undergoes compression between two porous transport layers (PTLs) during assembly [1]. Large deformations occur at the contact surface between the porous catalyst layer and the PTL fibers (Fig. 1, (a)).

Our work focusses on the influence of this deformation on effective transport properties. For that purpose, we numerically constructed Representative Volume Elements (RVE) as represenation of the microscale (Fig. 1, (b)). Based on this, a two-scale formulation using Variationally Consistent Homogenization (VCH) is derived. Previous numerical simulations have shown a significant non-linear reduction of the effective permeability during compression of the RVEs when considering fluid transport in the pore system. We examine, whether similar effects can also be observed for electronic and ionic conductivities in the electrolysis cell discussed above, which are important quantities for the overall electric performance. This is approached in two steps. First, we compute the fine-scale deformation of the RVE for a given macroscale deformation gradient. Second, a numerical study is performed on a set of sample RVEs with adopted fine-scale material properties to obtain effective conductivities.

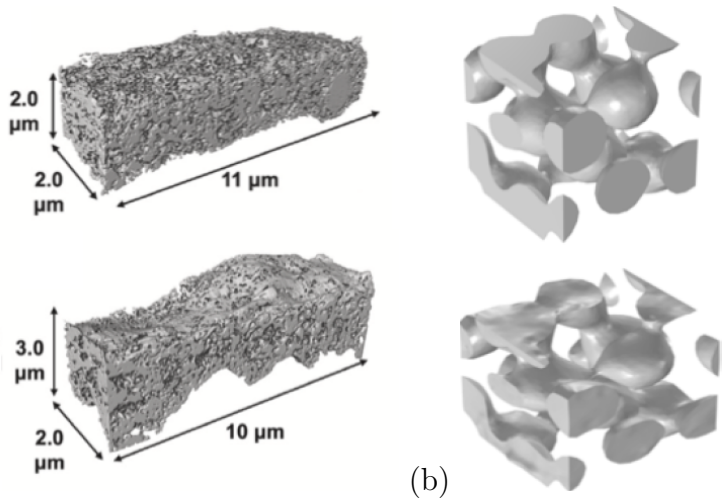

Figure 1: (a): PTL-fiber-compressed SEM reconstruction of catalysator layer before (top) and after compression (bottom) [2]. Large deformations are visible after compression. (b) Visualisation of corresponding deformed pore space in a numerical constructed RVE under a uniaxial compression.

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LEARNING ELASTOPLASTICITY WITH IMPLICIT LAYERS

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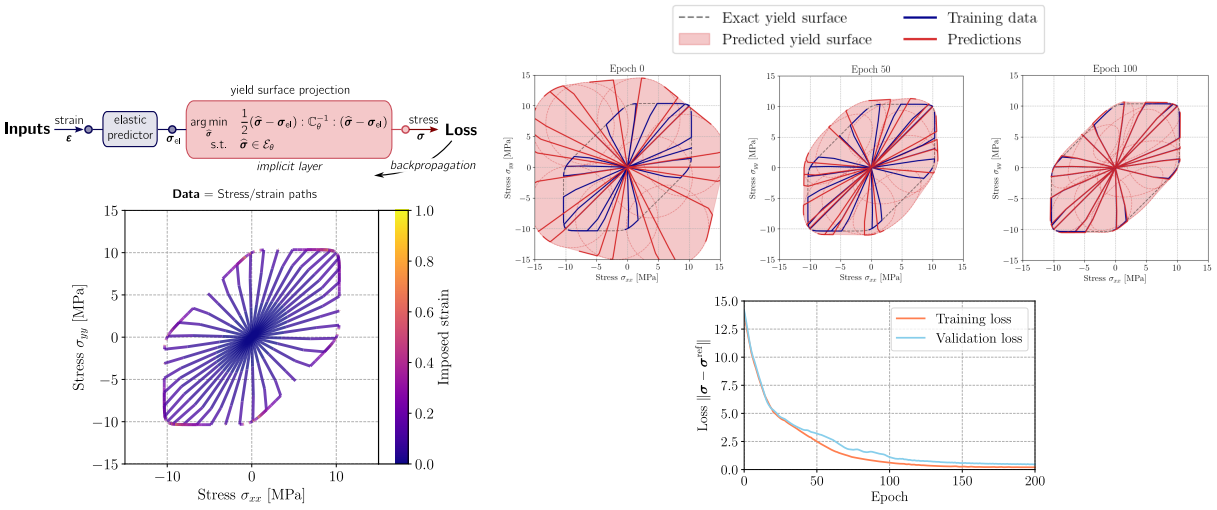
Key words: Data-driven, Plasticity, Machine Learning, Convex Optimization

Abstract. This work presents a novel machine learning approach for learning elastoplasticity directly from stress-strain data. Data-driven plasticity modeling is challenging due to the non-smooth transitions induced by the yield criterion and the complex nature of multi-dimensional yield surfaces. To address these difficulties, we propose an implicit layer-based architecture that formulates the elastoplastic constitutive update as a convex optimization problem with learnable parameters, representing general plastic yield surfaces as parametrized convex sets. The proposed approach exhibits strong generalization capabilities due to its embedded convex structure, achieving high performance even with limited data and in the presence of noise.

Most machine-learning (ML) models rely on explicit layers (e.g., perceptron, convolutional). In contrast, implicit layers [1, 2, 3] represent a fundamental shift, as they do not rely on sequences of matrix multiplications and predefined activation functions but instead solve optimization problems or implicit equations. Nonlinear constitutive laws share formal similarities with implicit layers. In some instances, a single implicit layer can be equivalent to an explicit deep net with infinite depth, offering large expressiveness with fewer parameters. However, this comes at the cost of increased computational complexity in evaluating the layer output.

This work explores the use of implicit layers to learn elastoplasticity and, in particular, plastic yield surfaces directly from data. For the sake of simplicity, we focus here on small-strain perfect plasticity (no hardening). For a given strain increment, the elastoplastic constitutive update is formulated as a convex optimization problem (see Fig. 1a) and the yield surface is represented as a parametrized convex set. The learning parameters $\boldsymbol{\theta}$ used to describe the elastic behavior and the shape of the plastic yield surface are then learned against existing stress/strain data.

Results on synthetic data corresponding to a biaxial stress/strain load paths on a Hosford yield surface (Fig. 1a) demonstrate the success of learning the elastic parameters



(a) Architecture and biaxial stress data

(b) Training results

Figure 1: Learning elastoplasticity with implicit layers.

and the plastic yield surface very efficiently. Training data uses only 20 load paths with 20 increments each. Validation is computed on 20 unseen load paths. Excellent generalization is obtained on unseen data owing to the underlying convex set approximation. Convergence is reached within only 100-150 epochs (Fig. 1b).

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A 3D MULTI-SCALE HYGRO-MECHANICAL MODEL OF OAK WOOD

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Key words: Oak anatomy, Level set-based image segmentation, X-FEM, Asymptotic homogenization, Moisture-dependent response

Abstract.

This contribution proposes a three-dimensional multi-scale framework for predicting the macroscopic hygro-elastic properties of (oak) wood by integrating the heterogeneous material characteristics from the nano-, micro-, and meso-scales [1]. The approach assumes a moisture-dependent constitutive description at the nano-scale, thereby recovering the moisture dependency of the material response at larger length scales.

At the macro-scale, oak wood is modeled as a homogeneous material. The meso-scale model derives from the cellular structure of individual growth rings, which include both the cell wall and the void regions, using detailed three-dimensional representations obtained via X-ray micro-computed tomography (μCT). These 3D meso-structural volumes, composed of voxel arrays with grayscale intensity values that reflect local material densities, are segmented using a level set–based method to distinguish cell walls from voids [2]. The resulting meso-scale phases are discretized using the extended finite element method (X-FEM). At the micro-scale, the heterogeneous nature of cell walls is captured by modeling the primary and secondary cell wall layers as a three-dimensional composite plate. Finally, at the nano-scale, the effective response is extracted from three-dimensional periodic unit cells consisting of cellulose micro-fibrils embedded in a matrix of hemicellulose and lignin.

The properties at the four scales are bridged through a three-level homogenization procedure (employing either an asymptotic homogenization or Voigt averaging approach as appropriate) to determine the effective hygro-elastic properties at the coarse scale. In addition, the moisture adsorption isotherms at each scale are constructed from a volume-weighted averaging of the moisture adsorption characteristics from the preceding scale.

The macro-scale hygro-mechanical behavior computed for oak growth rings agrees well with experimental data reported in the literature. Moreover, the meso-scale response

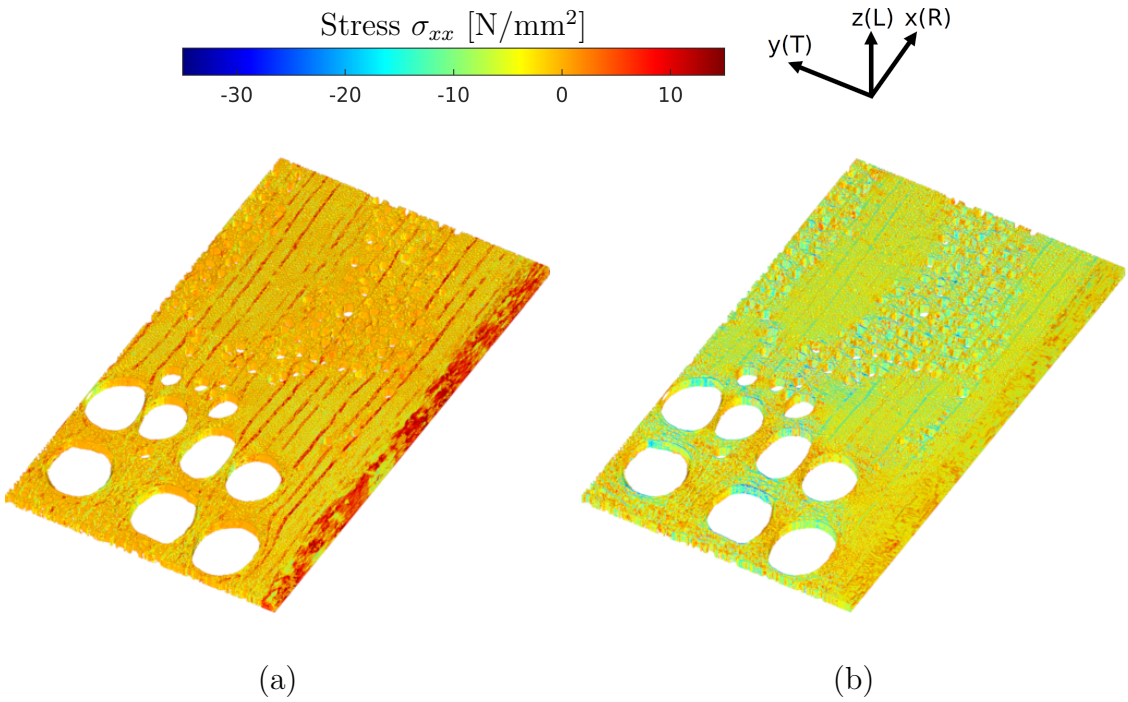

Figure 1: Meso-scale stress σ_{xx} in radial (R) direction in the oak growth ring under (a) *free expansion* and (b) *constrained expansion* conditions, computed for a moisture content variation $\Delta m = 1\%$ with respect to a reference moisture content $m_0 = 12\%$.

under representative moisture variations accurately identifies local, critical sites prone to mesoscopic hygro-mechanical damage - see Figure 1 [3]. The effective hygro-mechanical properties obtained through this multi-scale model can serve as an input for predicting the moisture-dependent mechanical response of oak wood structures subjected to arbitrary hygro-mechanical loading paths.

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A FFT-based approach for analyzing dissipation under low-amplitude cyclic loading in polycrystalline aggregates

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Key words: crystal plasticity, polycrystalline aggregate, dissipation, FFT methods, high-cycle fatigue (HCF), self-heating measurement

Abstract. The analysis of dissipation under cyclic loading, commonly referred to as self-heating measurements, is increasingly popular as a method for estimating the fatigue properties of materials in high-cycle conditions. The development of models linking self-heating measurements to fatigue properties is essential for exploiting the advantages of this experimental technique. This study proposes a method using the fast Fourier transform (FFT) applied to a representative volume element (RVE) of a polycrystalline aggregate to analyze the evolution of dissipation during low-amplitude cyclic loading and to construct predictive models. The approach emphasizes obtaining both qualitative and quantitative self-heating curves by analyzing how steady-state cyclic dissipation evolves under varying loading amplitudes. Uniaxial cyclic loading conditions are investigated. Particular emphasis is placed on the heterogeneous distribution of micro-plasticity within the polycrystalline aggregate, where dissipation is driven by localized plasticity in a small number of grains. This study also establishes connections with models using Poisson point processes to describe the gradual and localized emergence of these dissipation phenomena. Additionally, the investigation examines how several influence factors—such as grain orientation distribution, grain number, boundary conditions—affect the onset of dissipative phenomena within the polycrystal. The initial results are in good agreement with experimental data reported in prior studies.

A Sequential Approach for Topology Optimization of Coated, Manufacturable Structures

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Abstract

A sequential topology optimization framework is employed to design high-resolution, manufacturable coated structures by optimizing both the external boundary and the orthotropic infill. First, the Iso-XFEM method is utilized, incorporating the extended finite element method (XFEM) and a level-set approach to precisely define the design boundary. A coating layer of solid material with a fixed thickness is then introduced using morphological operations inspired by image processing techniques. Once the coated region is defined, a homogenization-based topology optimization method is applied to optimize the periodic microstructure of the infill. Following this sequential optimization process, a post-processing step maps the optimized microstructure onto a fine-scale mesh while ensuring the smoothness of the coated boundary. Numerical 2D examples demonstrate that this approach effectively generates coated structures with intricate features, enhancing structural performance and manufacturability through advanced additive manufacturing techniques.

Keywords: Topology optimization; Coated structures; Infill design; Homogenization; Additive-manufacturing

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A unified dual modeling framework for soft and hard magnetorheological elastomers: theory, computations and experiments

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Key words: Magnetorheological elastomers, dissipation, magnetoelasticity

Abstract. Most current magnetorheological elastomers (MREs) are broadly categorized into hard(h-MREs) and soft(s-MREs) depending on the magnetic properties of the underlying particles. The former consist of particles exhibiting strong magnetic dissipation (e.g., NdFeB), while the later are purely energetic (e.g., carbonyl iron). In this work [1,2], we present a unified modeling framework for h-MREs including the response of the s-MREs as a limiting case when the dissipation is set to zero. In addition, the proposed framework is dual in the sense of a partial Legendre-Fenchel transform of the magnetic part, i.e., we propose exactly equivalent models in the F−H and F−B variable spaces. Specifically, the models are capable of modeling the magnetic and the induced mechanical dissipation in the h-MREs, resulting from the ferromagnetic hysteresis of the underlying particles. In the limit of vanishingly small magnetic coercivity, both models yield a purely energetic response relevant for the s-MREs. Within the proposed framework, we show that the magnetization amplitude remains stretch-independent and we show experiments and numerical simulations to support this observation. We also connect the magnetization to an internal variable, thus indicating that extreme caution needs to be taken in the simplified case of purely energetic s-MREs and its use as an independent variable in the reference of current configuration. The proposed framework is also extended to include mechanical dissipation via finite strain viscoelasticity [3].

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Micromechanical modeling of metallic foams for power electronics converters

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Keywords: Metal foam, RVE, computational homogenization

Abstract. Reducing interconnection lengths in power electronic converters is crucial for enhancing efficiency and reliability. Open-cell metallic foams offer a promising solution, yet their full potential remains underexplored [1]. A key challenge is understanding how the foam's morphology influences its mechanical, thermal, and electrical properties, ultimately affecting converter performance. This study develops a computational framework to characterize these properties by generating numerical representative volume elements (RVEs) [2], and then applying computational homogenization to get their effective properties. A robust statistical approach is employed to determine the optimal RVE size, allowing control over the relative error in property estimation [3]. These insights provide a pathway for optimizing interconnections in power modules, potentially improving their performance and longevity.

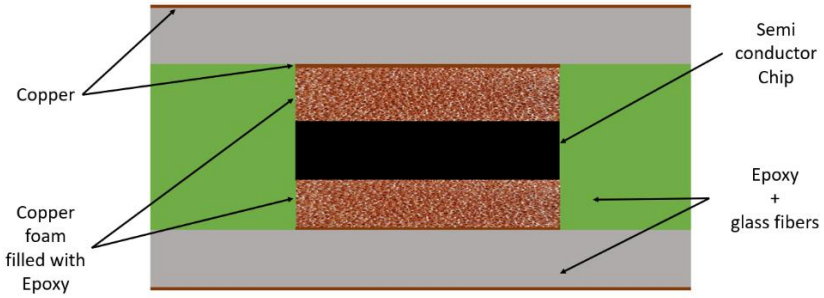

Figure 1: Illustration of open-cell metallic foam used to connect a semiconductor chip to a circuit board.

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FRACTURE IN CONCRETE: X-RAY TOMOGRAPHY WITH IN-SITU TESTING, DIGITAL VOLUME CORRELATION AND PHASE-FIELD MODELING

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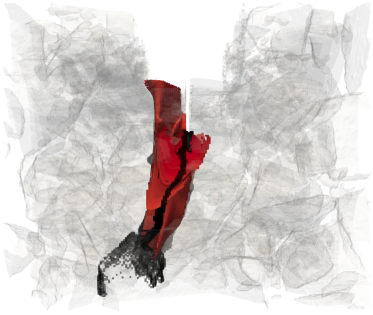
Key words: concrete fracture, digital volume correlation, phase-field modeling, in-situ testing, X-ray tomography

Abstract. We test and simulate the mesoscopic cracking behavior of specimens made of a standard concrete mixture. To this end, we combine stable wedge-splitting fracture experiments performed inside an X-ray tomograph, their analysis with digital volume correlation providing the full three-dimensional displacement field, and phase-field fracture modeling. In our computations, we apply the measured boundary conditions and model the actual heterogeneous material structure at the concrete mesoscopic scale. Within the phase field model, we explicitly distinguish among (thus individually represent) the mesostructural features of distinct material phases with size above a threshold of 1 mm, while we homogenize pores and finer aggregates below this threshold within the cementitious mortar matrix, with material parameters characterized accordingly. We compare experimental and numerical results in terms of both local and global quantities.

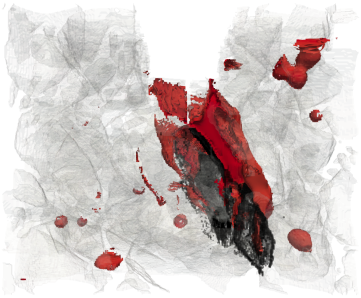
Figure 1 shows the experimental and computational crack patterns for the three specimens, of which the first two exhibited the expected failure mode (were split open by a crack propagating from the initial wedge downwards), whereas the third failed by a lateral crack, which was induced by the specific mesostructure and captured by the computational predictions. For many more details, see [1].

(a) Specimen #1, front view

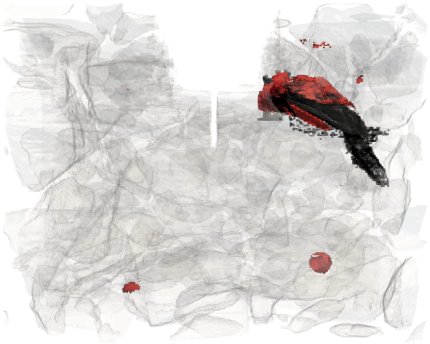


(b) Specimen #1, back view

(c) Specimen #2, front view



(d) (b) Specimen #2, back view



(e) Specimen #3, front view

(f) (b) Specimen #3, back view

Figure 1: Experimental (black) and computational (red) crack patterns.

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INVESTIGATING DAMAGE AND PLASTICITY IN RC NUCLEAR FACILITIES UNDER SEISMIC LOADING

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Key words: Damage, Plasticity, Numerical homogenization, Reinforced concrete

Abstract.

Reinforced concrete (RC) structures in the nuclear field are subject to stringent regulations, particularly for seismic demands. Understanding RC behavior under mechanical loads especially during earthquakes, and modeling this behavior numerically is crucial for assessing the robustness and safety of the structures and the hosted equipment, both at the design and reassessment stages. Our research focuses on developing a multi-layer, multi-material finite element plate model designed for large-scale simulations of RC structures in nuclear facilities and capable of representing engineering key quantities such as the floor spectra and the energy dissipation. The model aims to reflect the effects of microscopic non-linearities at a macroscopic level: the top and bottom layers in the thickness of the RC plate will be modeled as an equivalent homogenized material representative of the steel grids, the surrounding concrete, and the interface between the two materials; while the core will be modeled using a non-linear damage model for concrete. The model will strive to strike a crucial balance between accurately representing the complex material behavior and ensuring computational efficiency, practical usability, and parameter calibration. A simple rheological model representative of a 1D reinforced concrete tie has been analyzed under various load conditions to assess the role of different modeling assumptions on global and local responses. The results, validated using experimental

references, have confirmed the necessity of including the non-linear interface in numerical models for RC and have emphasized the need for a comprehensive understanding of non-linear phenomena and their interactions. These initial results have been extended to the study of a Representative Elementary Volume (REV) representative of the top and bottom layers of an RC plate, including the steel bars, the surrounding concrete, and the interface. The REV has been tested under various loading conditions and the collected results will be integrated in the homogenization process that will be conducted in the linear elastic framework, at fixed values of the internal variables and integrating the effect of the steel-concrete interface [1][2][3].

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MODELING AND NUMERICAL UPSCALING OF TEXTILE REINFORCED CONCRETE PLATES

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Key words: Computational homogenization, Textile reinforced concrete

Abstract. In this work we propose a numerical homogenization scheme that can be used to model textile reinforced concrete (TRC) on the macro scale using an effective plate model

Textile reinforced concrete (TRC) is an emerging material that utilizes fiber textiles instead of steel as reinforcement. TRC offers two key advantages over steel reinforced concrete (RC): it is corrosion-resistant and the reinforcement has higher specific tensile strength. When applied correctly, these benefits can significantly reduce the CO_2-eq emissions compared to RC.

TRC has not yet been widely adopted, partly due to the lack of comprehensive mechanical models for design and analysis. To address this gap, this work presents a comprehensive upscaling framework from the meso to macro scale. In this framework, representative volume elements are employed to model the resolved concrete and reinforcement on the meso-scale. The bond and interfilament slip are captured by a one-dimensional bond-slip model and efficiency factors for stiffness and strength, that have been calibrated in [1]. Additionally, cracking and crushing of the concrete are modeled using the Mazars damage model. The upscaling is performed using Variationally Consistent Homogenization (VCH), where the prolongation and homogenization mappings are derived for the Kirchhoff-Love plate kinematics.

The proposed method is validated through comparison to direct numerical simulations and analytical solutions, demonstrating its ability to accurately approximate the effective membrane forces and bending moments of a TRC plate.

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SURROGATE POROUS MICROSTRUCTURE GENERATOR: APPLICATION TO TRISO NUCLEAR FUELS

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Key words: Surrogate Modeling, Gaussian Random Fields, Homogenization, Nuclear Fuels

Abstract. The aim of this work is to provide a surrogate microstructure generator for porous materials and to compare homogenized mechanical predictions of the surrogate microstructure with the one obtained from measured microstructure data.

The surrogate model is constructed using a level-set approach combining a regular microstructure (called the *topological support*) with a noise field (based on a *Gaussian Random Field/ GRF*), building on the work in [1]. The aim of the construction is to represent random morphological features of the microstructure. More over the topological support is constructed of a series of elliptical inclusions which are eventually clustered in order to catch up the complex shapes of the pores. Irregularities at the pore surface are created by the intersection with the GRF. Parameters characterizing the microstructure are identified using a stochastic optimization procedure from morphological images by minimizing a cost function, which embodies several statistical and geometrical distances of the morphology. Finally the elastic and damage prediction of surrogate and measured microstructures are compared over a series of elementary representative volume elements, using the AMITEX FFT library.

The viability of the approach is demonstrated through the application to the porous pyrocarbon buffer layer of *tristructural isotropic* nuclear fuel (TRISO) [2].

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MODELING INTERGRANULAR DAMAGE ASSISTED BY OXIDATION IN NICKEL-BASED SUPERALLOYS

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Key words: Nickel-based superalloys, Phase-field modeling, Intergranular damage, Creep modeling

Abstract. Nickel-based superalloys, such as the DS200+Hf, are extensively used in high-temperature components of aerospace turbines, particularly for low-pressure turbine blades in CFM-56 and LEAP engines [1]. These alloys generally feature a columnar grain structure with the main grain axis closely aligned with the principal loading direction (e.g., centrifugal forces in rotating components). Furthermore, the directional solidification process ensures that the main grain axis is typically near a [001] crystallographic orientation.

This study focuses on modeling the mechanisms of intergranular damage in the directionally solidified DS200 + Hf superalloy, considering local phenomena such as cracks, microcavities, and oxidation, which critically influence the initiation and propagation of intergranular cracks. The damage evolution was examined using finite element simulations and experimental data [2], with the microstructural characteristics, including grain size and texture, determined through electron backscatter diffraction (EBSD) analyses.

To capture these complex phenomena, a novel phase-field method for fracture modeling in polycrystalline materials was developed. Numerous studies have addressed this issue by incorporating cohesive models at grain boundaries [3, 4]. However, these models often face convergence challenges, particularly in complex surface geometries. Musienko *et al.* [5] proposed an alternative approach, defining grain boundaries through a viscoplastic model with damage, implemented using a specifically designed mesh to represent grain boundaries with a finite thickness. While this model demonstrates good convergence, it introduces a sharp transition in behavior between the grains and the grain boundaries. To address these limitations, the phase-field model offers a versatile framework with an internal length scale tailored for systems with sharp interfaces. Nguyen *et al.* [6, 7] proposed a phase-field approach for polycrystalline materials, where interface failure is

governed by a cohesive law embedded within a regularized variational framework. The interfaces in their model are captured using a level-set method.

The present study focuses on developing a model that excludes the influence of oxidation. This model is built on the finite strain framework and integrated into the Méric–Cailletaud model, employing a two-potential approach for low strain rates and high strain rates to capture crystalline viscoplasticity at the grain level. The model is enhanced with a static phase-field method, enabling the distinction between grain boundaries and grains through a diffuse interface representation. Additionally, a Lemaitre-type damage law is incorporated to describe the evolution of damage, including deformation mechanisms induced by damage. This model is implemented in the finite element code Z-set, with both explicit and implicit resolution.

The model was validated through simulations of creep and tensile tests, with results compared to experimental data obtained under vacuum conditions. The findings highlight the model's ability to replicate the nucleation and propagation of intergranular cracks, offering valuable insights into the damage mechanisms of directionally solidified superalloys.

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DARK ENERGY IN CRYSTALS: PREDICTION OF STORED ENERGY AND IMPACT ON RECRYSTALLIZATION

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Key words: Crystal plasticity, Stored energy, Cosserat media, Phase field

Abstract.

During the plastic deformation of metallic materials, part of expended mechanical work diffuses as heat. The fraction of plastic work converted into heat is called the Taylor–Quinney Coefficient (TQC), which is often assumed to be a constant parameter of about 0.9. The remaining portion of the plastic work is called stored energy. The stored energy is known as the main driving force for dynamic or static recovery and recrystallization. Therefore, numerical predictions and experimental measurements of the stored energy and TQC are essential to optimize thermomechanical material processing. In this work, a thermodynamic class of crystal plasticity models is used to predict the stored energy and TQC of copper and aluminum single crystals. Then, the numerical stored energy predictions are extended to polycrystalline austenitic steel 316L and compared with the experimental measurements from the literature. The contributions of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs) for the stored energy prediction are taken into account using strain gradient crystal plasticity. The presented computational analysis indicates that, compared to the experiment, there remains dark energy in the evaluation of energy storage as predicted by the proposed thermodynamically consistent crystal plasticity framework [1].

The evaluated stored energy density is then used as a driving force in a combined Cosserat mechanics-phase field model of grain boundary migration and recrystallization [2, 3]. In the numerical simulation of these processes, grain nucleation is generally treated as an additional ad hoc step in which circular or spherical grains are added in regions where a critical dislocation density, stress or strain are reached. In contrast, systematic finite element simulations are performed showing that the Kobayashi–Warren–Carter (KWC) phase field model predicts spontaneous nucleation of new grains in single crystals in the presence of lattice orientation/rotation gradients. The numerical analysis of

the stability of gradients of lattice rotation and dislocation-based stored energy indicates that a gradient of stored energy alone is not sufficient to trigger grain formation. As an application, the KWC–Cosserat model is used to simulate the torsion and annealing of a copper single crystal bar with a circular cross section. This mechanical loading produces a large, fairly uniform axial rotation gradient which induces nucleation in the form of a stack of cylindrical grains, as confirmed by experimental observations from the literature.

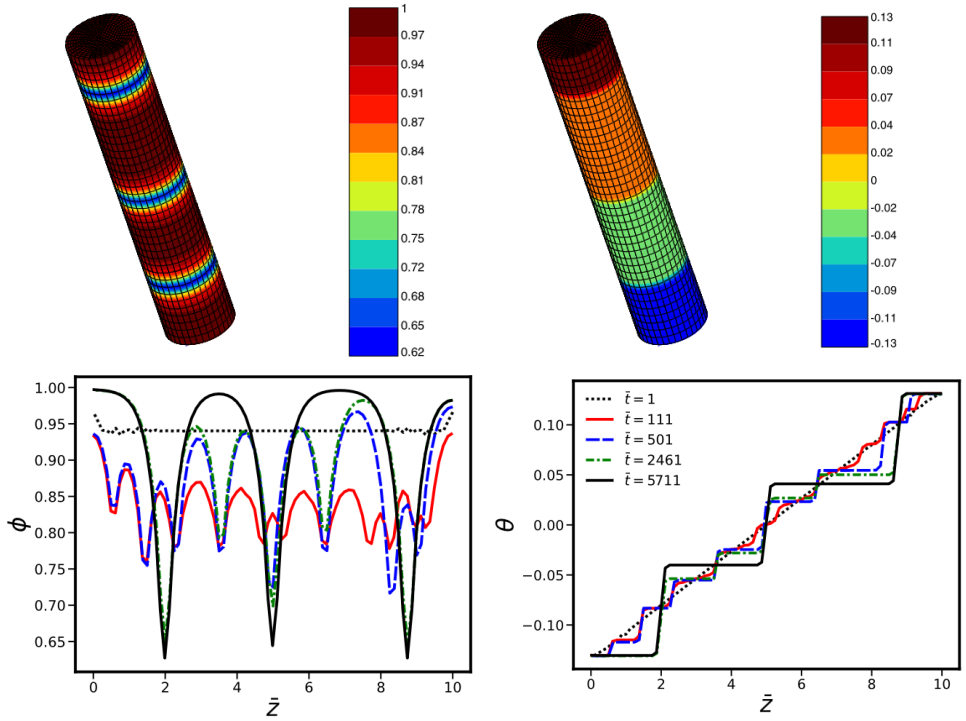

Figure 1: Grain nucleation in a single crystalline bar in torsion: phase field and lattice orientation in the bar (top), and along the axis at successive time steps [3].

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THERMO-PLASTIC NONUNIFORM TRANSFORMATION FIELD ANALYSIS

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Key words: nonlinear elasto-thermo-plastic homogenization, Nonuniform Transformation Field Analysis (NTFA)

Abstract. The rigorous and efficient homogenization of elasto-thermo-plastic materials is a long-standing problem: Besides the intrinsic path-dependency of the material, the elastic behavior can vary drastically with changes in temperature. In order to tackle this problem we extend the Nonuniform Transformation Field Analysis (NTFA) to materials with evolving elastic properties. This is achieved by inserting an intermediate affinely linear reduced order model to obtain the temperature dependent interaction tensors of the NTFA. The efficiency and accuracy of the original NTFA is obtained even if the temperature of metal matrix composites is varied from room temperature to close to the melting temperature. We demonstrate the capabilities of the resulting reduced order model in twoscale simulations.

Three decades ago, Dvorak [5] presented a micro-mechanically rooted approach to the homogenization of inelastic composite materials by means of the Transformation Field Analysis (TFA). It has paved the way for an entire class of scale-bridging methods. The core idea of the TFA is the recourse to piece-wise constant transformation fields. It turns out that within each sub-domain, the driving forces for plastic deformation boil down to a linear mapping of the mode activity. The obvious shortcomings of piece-wise uniform transformation strains have led to the Nonuniform Transformation Field Analysis (NTFA) originally proposed by Michel and Suquet [4], and with several additions by the author (e.g., [3]). The NTFA is capable of reducing the nonlinear path-dependent problem to a modest number of plastic internal variables on the larger scale, although the model is completely microstructure-informed.

A major shortcoming of the NTFA remained its reliance on constant elastic properties and, therefore, constant interaction tensors that link the new state variables to the driv-

ing forces. In thermo-plastic materials, this assumption can however not be kept alive: Besides manageable thermal eigenstresses, the elastic constants of metals can change substantially if the temperature changes are non-negligible. To cope with such variations we propose a novel Thermo-plastic NTFA (θ-NTFA) in [1]. The main challenge is the solution of auxiliar linear problems given thermo-plastic eigenstrains as a function of the temperature θ. The use of classical numerical techniques such as the finite element method (to be solved for each temperature θ) must be discarded due to the related numerical investment, resulting in the need for robust and accurate surrogates for this intermediate step. For this step, we rely on affinely linear reduced order models that we developed for thermo-elastic homogenization in [2]. As a result, numerical high-fidelity simulations of the eigenstrain problems are needed at some 5 to 10 discrete temperatures only to accurately cover the full span from 20 to 1000°C in copper-tungsten carbide composites. In view of the applicability of the method, the intermediate reduced order model is inexpensive to evaluate, but technically involved. Therefore, we decided to tabulate the temperature dependent interaction tensors, e.g., at 1000 intermediate temperatures. The resulting NTFA model then boils down to a linear interpolation of the interaction tensors from this database followed by a classical NTFA implementation [1].

An application of the θ-NTFA is the process simulation of laser melt injection generated surface reinforcements. The goal is to understand the eigenstresses in the tungsten carbide particles and the tractions on the particle surface in such composites which are experimentally inaccessible. Therefore, the simulations are the only available tool to gain insights into potential causes for damage. Our work emphasizes the versatility of micro-mechanically inspired (N)TFA-based approaches over purely data-driven schemes.

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MULTISCALE ANALYSIS OF THE ANISOTROPY INDUCED BY LPBF DEFECTS WITH COARSE GRAINING

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Key words: Additive manufacturing, LPBF, Defectology, Anisotropy, Coarse graining, Simulation on images.

Abstract. Laser Powder Bed Fusion (LPBF) additive manufacturing offers interesting possibilities for numerous industrial applications. However, this process can also generate defects whose criticality can, if not controlled, significantly affect the durability of structures. This study proposes a method to establish a direct link between the spatial distribution of porosities and the induced anisotropy of the material at different scales. It uses multigrid image simulations and a coarse graining (CG) homogenisation technique.

Additive manufacturing techniques have garnered significant interest in various industrial applications due to their potential for design optimisation, cost reduction, and shortened lead times. Among these techniques, Laser Powder Bed Fusion (LPBF) stands out for its ability to produce components with satisfying material properties and complex designs unachievable with traditional manufacturing processes. These features are also relevant in the nuclear industry and particularly for reactor internal components which are highly solicited in very restricted spaces [1].

Despite its benefits, this technique also presents a specific defectology characterised by the type and quantity of pores, their spatial distribution and the interactions between them. It can be strongly influenced by the numerous manufacturing parameters, including the powder characteristics, the laser path and specifications, or the complex interactions between these factors. In particular, a strong correlation can be observed between the lasing strategy used and the location of defects, revealing signature patterns [2] that could affect the symmetry group of the homogenised material. Besides, since pore populations are highly diverse and the components typically fine, the existence or the appropriate size

of a Representative Volume Element (RVE) remains uncertain. Moreover, with the thin designs enabled by LPBF, the defect size can approach the structure scale which raises the question of the validity of the scale separation hypothesis in homogenisation.

In this work, we study the anisotropy induced by the particular spatial organisation of complex defect populations and investigate the existence of a homogenised RVE for such materials.

We address this question by performing high-fidelity multigrid elastic simulations on synthetic images representing a given distribution of pores [3]. Elastic computations are conducted using six independent loading cases (KUBC) to evaluate the elasticity tensor.

Coarse graining (CG) is used to perform an exact homogenisation of the domain at multiple scales [4]. In this approach, the mesoscopic variables are computed from the convolution of microscopic variables with a kernel, while enforcing mechanical conservation laws at both scales. As a result, the method provides homogenised property fields across all elements without the need of a RVE. It is also worth noting that no assumptions are made regarding the material's behaviour. Thus, the elasticity tensor can be evaluated at multiple mesoscopic scales. The number of independent eigenvalues of the elasticity tensor is then used as an indicator of the local anisotropy degree of the homogenised material.

Therefore, CG techniques allow for establishing correlations between the microscopic defect distributions and the resulting elastic properties at different scales. These findings highlight the anisotropy induced by defects depending on the observation scale considered. Furthermore, the analysis of the variability of the homogenised elastic properties at different scales enables conclusions regarding the existence or size of a RVE and its degree of anisotropy.

Currently, the approach shows promising results in capturing anisotropic behaviours induced by voids at mesoscopic scales for relatively simple cases. Future work will focus on investigating the existence or size of a RVE and applying the same scheme to more complex defect populations. The validity of the scale separation hypothesis should also be examined.

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THE MIMINUM ENERGY ATOMIC DEPOSITION METHOD FOR THIN FILM GROWTH AND MECHANICS

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Key words: atomic deposition, minimum energy, thin films

Abstract. This contribution focuses on the Minimum Energy Deposition Method as a versatile tool for thin film growth and the evolution of physical and mechanical fields during thin film deposition.

Thin-film growth is an area of research concerned with complex phenomena happening at atomic scales. Therefore, molecular simulations constitute an important tool to confront experimental results to theoretical assumptions. However, the traditional thin film growth simulation methods, i.e., Molecular Dynamics (MD) and kinetic Monte-Carlo (kMC) and combinations thereof, suffer from some intrinsic limitations, i.e. limitations in system size and simulation time for MD and predetermined reaction rates and reaction sites for kMC. Consequently, it is practically impossible to simulate the evolution of polycrystalline growth resulting in ≈100 nm thick films with realistic stress fields and defect structures, such as grain boundaries, stacking faults, etc.

This contribution presents an extremely simple and computationally efficient atomistic simulation method (Minimum Energy Atomic Deposition: MEAD) to simulate thin-film deposition [1]. The method aims to overcome the limitations of existing methods to enable

in-depth studies of atomic growth mechanisms, the evolution of crystal defects, and residual stress build-up during thin-film deposition—an important and active research area. The method allows depositions of tens of millions of atoms at near-equilibrium deposition rates in reasonable computational time while allowing for the growth of >100 nm-thick films with high crystallinity and low defect concentration. This has been validated on three material systems (the deposition of Al on Si, Al on Al, and Si on Si), demonstrating that the method is much faster than MD simulations. However, the proposed method does not aim to replace the existing algorithms such as MD or kMC, but instead, improve upon the existing methods in certain aspects by integrating them into the MEAD method. One can combine the MEAD algorithm with existing techniques such as energy minimization with FIRE, thermal equilibration with tfMC, and MD equilibration, thereby also incorporating the capabilities of these techniques. Unlike on-lattice kMC, the method does not need pre-determined reaction rates and deposition sites—both of which naturally emerge from the simulation methodology. The presented results are also coherent with the experimental literature on thin film deposition. Hence, this method can be broadly used to simulate and analyze the evolution of defect structures and the build-up of residual stress during thin film growth and subsequent heat treatments. The use of in-built functions in LAMMPS makes the method easily accessible to the community.

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MICROSCOPY-INFORMED PROBABILISTIC MULTISCALE MODELING OF CARBON NANOTUBE POLYMER COMPOSITES

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Key words: Carbon nanotubes, Multiscale modeling

Abstract. Advanced materials development increasingly relies on hierarchical modeling integrating microstructural data from imaging techniques for accurate microstructural representation with observed properties across nano- to large scales. One key challenge in developing these models is to strike a balance between computational efficiency and predictive accuracy while addressing uncertainties in input parameters, microstructure, and interfacial properties.

This paper presents a probabilistic bottom-up multiscale framework for predicting the mechanical properties of carbon nanotube-filled polymer composites (Figure 1). The framework leverages 2D and 3D image characterizations from transmission electron microscopy (TEM) and confocal laser scanning microscopy (CLSM) to inform the construction of representative volume elements (RVEs) at nano- and microscales. It integrates probabilistic modeling, considering probabilistic distributions of parameters such as aggregation number (N), waviness (α), orientation (θ), and filler weight fraction (w_f). Molecular dynamics (MD) simulations at the nanoscale inform the mesoscale and macroscale models, with micromechanics theories like Mori-Tanaka (MT) and finite element analysis (FEA) employed for upscaling. Additionally, variance-based sensitivity analyses are used to evaluate the influence of uncertain input parameters. Monte Carlo sampling is used to generate input parameter spaces, and sampling efficiency is enhanced by the Saltelli method. Simulations across sample sizes (n = 10,000–3,000,000) confirm convergence for first- and total-order sensitivity indices, with higher-order interactions reported at larger sample sizes. The sensitivity analyses provide insights into dominant factors and their interactions, which are critical for optimizing the multiscale modeling framework.

The results demonstrate the efficiency and accuracy of the multiscale model in predicting the mechanical properties of CNT-filled nanocomposites. Statistical analyses of CLSM and TEM images confirm that filler orientation, waviness, and volume distributions follow normal distributions, contributing to input parameters for the model. Sensitivity analyses reveal that waviness, orientation, and weight fraction significantly influence the longitudinal elastic modulus, while aggregation number has negligible impact. At the nanoscale, custom hyperplanes provide better predictions of elastic properties than polynomial hyperplanes, though *R*-squared values are limited for shear modulus and Poisson's ratio due to in-plane and out-of-plane randomness. Microscale results show that aligned fillers maximize longitudinal elastic modulus, with waviness reducing its effect at higher weight fractions. At the macroscale, predictions using MT theory and FEA reveal linear increases in mechanical properties with filler weight fraction.

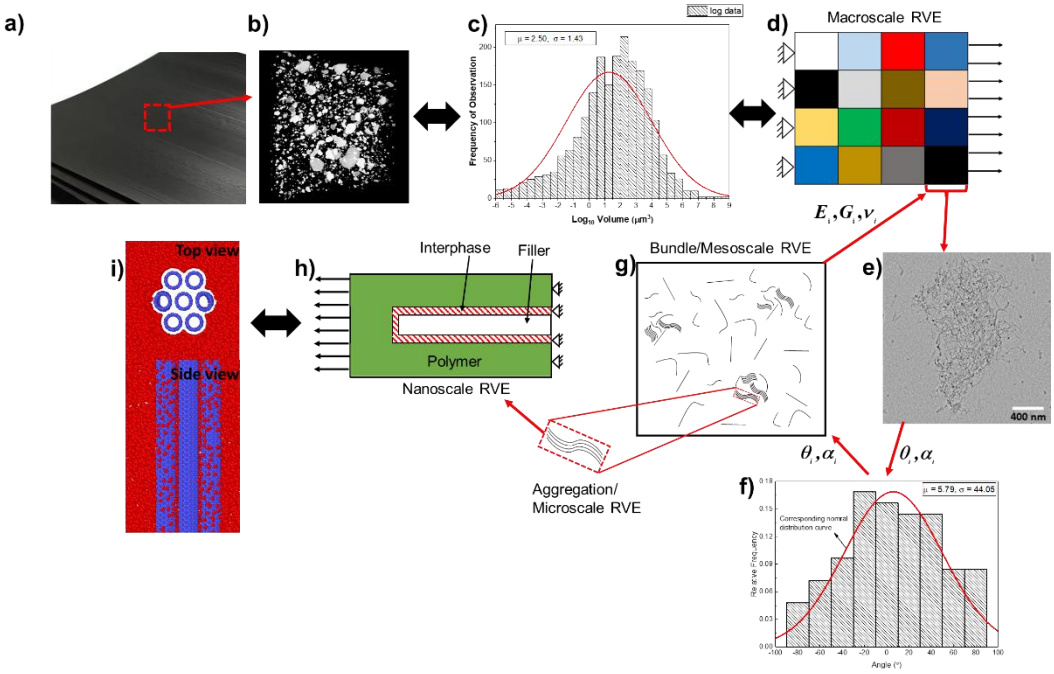

Figure 1: The bottom-up multiscale modeling scheme of CNT-filled nanocomposites: a) a nanocomposite reinforced with CNT, b) a CLSM image of sample at macroscale, and c) volume distribution of embedded CNT bundles in CLSM image [1], d) a macroscale RVE made of many mesoscale RVEs representing CLSM image. Each mesoscale RVE contained e) a bundle of CNT captured by TEM and f) corresponding orientation distribution of the CNTs and their aggregations in that bundle. g) constructed mesoscale RVEs and h) nanoscale RVEs for MD simulations.

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IN-SILICO DESIGN OF ELECTRO-ACTIVE POLYMER BASED SOFT ROBOTICS: STABILITY, MULTI-SCALE MODELLING AND ENHANCED GAUSSIAN PREDICTORS

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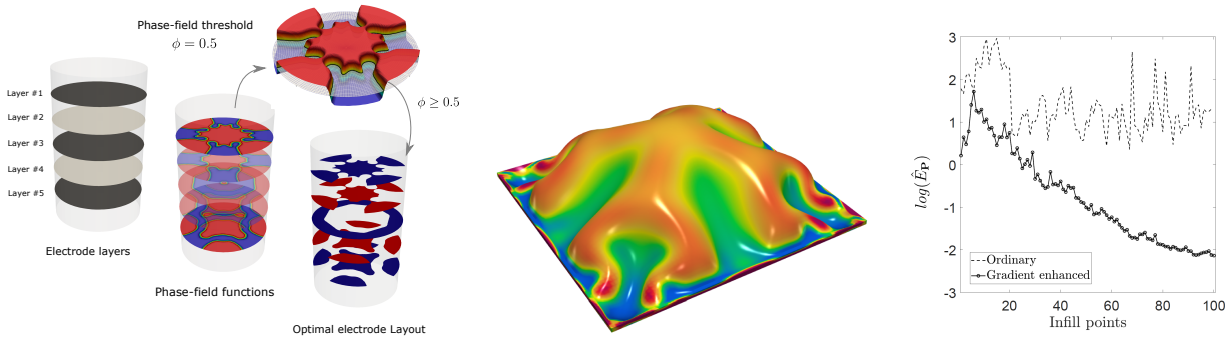
Key words: Electroactive Polymers, Stability, Topology Optimisation, Rank-one Laminates, Multiscale, Soft Robotics

Abstract. The use of Electro-Active Polymers (EAPs) for the fabrication of evermore sophisticated miniaturised soft robotic actuators has seen an impressive development in recent years. This contribution will unveil the latest computational developments of the group related to some significant challenges in the in-silico modelling of EAPs, which include (i) robustly resolving the onset of potentially massive strains and instabilities; (ii) optimising the meso-architecture to enable device customisation for specific application required deformations; and (iii) accurately capturing the properties of multi-phased composites at a macroscale level.

The field of soft robotics is focused on exploiting smart (or animate) materials capable of rapidly reacting and adapting to their environment. Electroactive Polymers (EAPs) are a particular subclass of smart materials activated via an electric field which exhibit sought after properties including high energy density, rapid rate of response, and low weight. This contribution showcases a novel in-silico tool [1, 3] for the design of complex multilayer EAPs characterised by layer-by-layer reconfigurable electrode meso-architectures. The ultimate objective is to help thrive the development of this technology through the in-silico (Topology Optimisation) production of voltage-tunable EAPs beyond those obtained solely via trial-and-error experimental investigation.

Leveraging the whole spectrum of EAPs' functionalities requires of sophisticated microstructures incorporating micro-scale lamination [2] or inclusions. To model the device

level macro-scale responses from these complex microstructures, multi-scale homogenisation modelling strategies must be utilised. In addition to a classical multi-field Finite Element Method FEM^2 homogenisation approach, a new Physics Augmented Machine Learning (ML) will be presented to drastically reduce online computational costs. Gaussian Predictors [4, 5], due to their ability to provide metamodel uncertainty, calibrate on small datasets, and exploit gradient (noisy) data and uncertainty-based infill strategies, will be the method of choice.



(a) (b) (c)

Figure 1: (a) Topology optimisation of EAP meso-architecture. (b) EAP onset of wrinkling. (c) Gradient Enhanced Gaussian Predictor improved convergence.

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COUPLED PHASE FIELD CRYSTAL AND FIELD DISLOCATION MECHANICS: A NEW CRYSTALLOGRAPHIC DISLOCATION MECHANICS APPROACH

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Key words: Dislocations, Phase field, Elasticity, Plasticity, Numerical methods

Abstract. The Phase Field Crystal (PFC) is a modeling approach for crystalline materials over diffusive timescales. It naturally captures stable topological defects such as dislocations. However, due to its diffusive evolution, it struggles to accurately handle elasticity. The aim of this work is to couple PFC with Field Dislocation Mechanics (FDM) to incorporate elasticity within the phase field evolution. FDM is the state-of-the-art theory for modeling dislocation mechanics, but it fails to naturally maintain compact dislocation cores due to a general lack of crystallography in its formulation. The resulting coupled PFC-FDM framework between these two complementary theories overcomes their individual limitations and provides a pathway for modeling elasto-statics, dynamics and interactions of crystallographic dislocations at diffusive timescales. In this work, the finite element based numerical implementation of the strongly coupled PFC-FDM model is first presented, followed by the demonstration of the advantages of this coupling in predicting dislocation statics and dynamics.

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DATABASED MULTI-SCALE TOPOLOGY OPTIMIZATION OF ARCHITECTURED MATERIALS

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Key words: architectured materials, multi-scale topology optimization

Abstract. With respect to increasing industry demands for predictable computer simulations, the development of numerical methods in structural design has received considerable attention over the past few decades. Among them, the optimization of the topology has proven its effectiveness for the design of complex structures with requirement of specific mechanical properties. The latest advances in 3D printing processes allow today to manufacture of sophisticated structures and micro-architectural materials. This work presents an original approach for the design of compliant mechanisms integrating micro-architectured materials based on a multi-scale strategy. The underlying idea is that micro-architectured materials may exhibit more complex behaviors compared to standard materials. Therefore, adding those materials in the design of compliant mechanisms can lead to better performance. The method used replaces the standard density distribution used in common topology optimization methods, such as SIMP or levelset methods, by a distribution of material properties. Once the optimization has converged, a material map of the properties in the design domain are obtained and the corresponding microstructures are designed a posteriori by inverse homogenization. However, the computational cost associated with such a method can become exorbitant, especially if the number of micro-architectured materials to be designed is substantial. A databased approach is studied to reduce these computational efforts. An optimized catalog of micro-structured materials covering a wide range of different mechanical behaviors is calculated a priori. The catalog is then consulted to extract the micro-architectured materials as closely as possible, in terms of mechanical behaviors, compared to what is required for the compliant mechanism [1, 2, 3, 4].

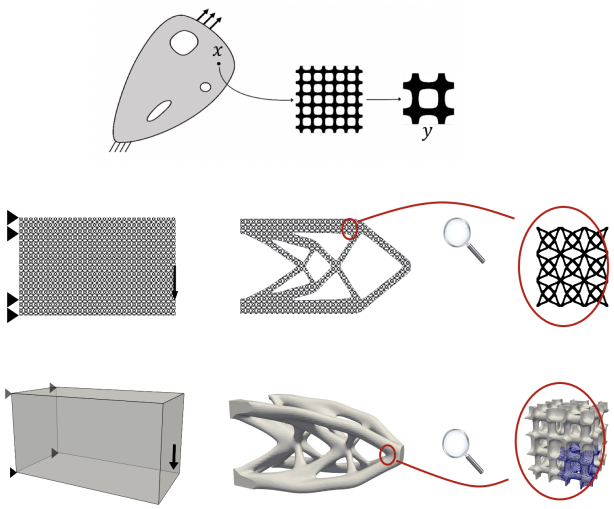

Figure 1: Multi-scale optimization of architectured structures.

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PROBING DUCTILE DAMAGE MODELS WITH RANDOM POROUS METAMATERIALS

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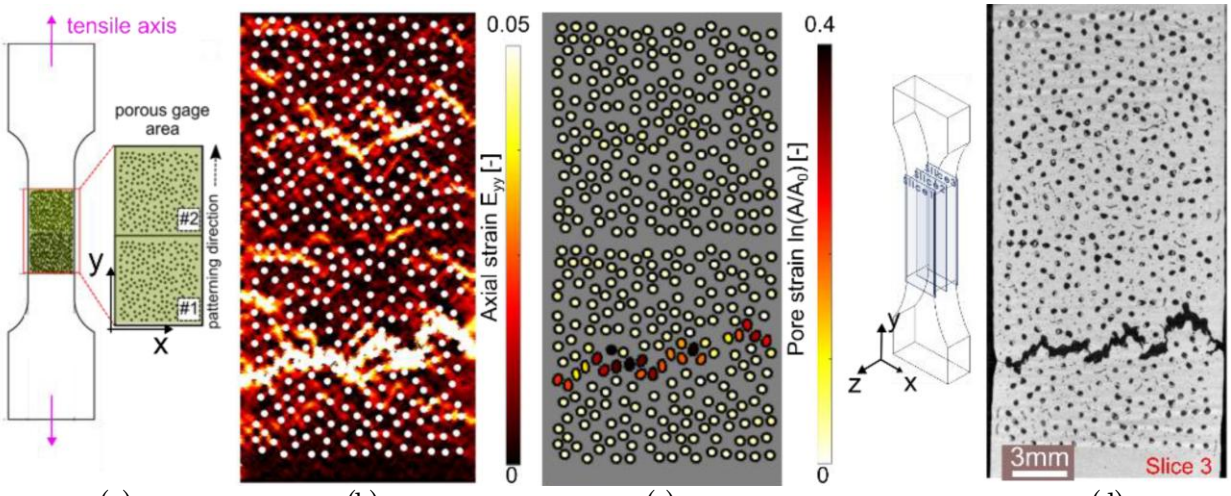
Key words: Aluminum alloy, Full-field measurements, Identification, In situ experiment

Abstract. Ductile fracture is the most common room temperature failure mechanism in metals and alloys. It results from the nucleation, growth and coalescence of microscopic voids embedded in metallic matrices. The subject now comprises a vast body of theoretical and experimental work [1]. Yet, while significant progress has been made, several open questions still remain. One concerns the competition between plastic localization and damage.

In this work, ductile damage was probed at the mesoscale using additively-manufactured porous metamaterials. The metamaterials of this study had a porous architecture in which cylindrical pores, of arbitrary elliptical shape, were randomly-dispersed in an AlSi10Mg matrix (Figure 1(a)). Their porous architecture was generated numerically by means of a random sequential absorption algorithm and was fabricated by laser powder-bed fusion (LPBF) [2].

Using FE-based Digital Image / Volume Correlation (DIC / DVC) with mesoscale meshes consistent with the pore distribution enables for kinematic measurements at the mesoscale (Figure 1(b)). With such data, it was possible to assess the pore strains, which are defined as the logarithm of the current pore surface divided by its initial level (Figure 1(c)). These observations are consistent with the post-mortem observations performed via computed tomography (Figure 1(d)). The previous data can then be directly compared to damage predictions [2] (e.g., using McClintock's model [3]).

DVC analyses can also be combined with numerical simulations [4]. It is then possible to calibrate nonlinear models at the mesoscale [5]. Void growth and coalescence (during in situ tensile straining) were also quantified for this class of cellular solids. Different strategies were used to calibrate the parameters of a Voce hardening law for the matrix. It is shown that the damage process was dictated by the interactions between the cylindrical voids and were significantly promoted by the presence of manufacturing defects, which inevitably formed within the matrix.



(a) (b) (c) (d)

Figure 1: (a) Mesoporous architecture. (b) Longitudinal strain field measured via FE-based DIC. (c) Corresponding pore strain field. (b) Section of post-mortem scan of the sample

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SYMMETRIES OF HETEROGENEOUS MATERIALS: FROM INVARIANCE TO INDISTINGUISHABILITY

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Key words: Architectured materials, Point group, Quasiperiodicity, Indistinguishability, Fourier transform

Abstract. We present a method to detect the point group symmetries of a microstructure based on the criterion of indistinguishability.

The effective behaviour of multiscale materials is governed by the arrangement of matter at the microscale. If this microstructure is deterministic, i.e. periodic or quasiperiodic, its point group symmetries manifest in its effective linear behaviour by determining the symmetry class of effective tensors.
In the case of periodic microstructures, the point group is defined as leaving the microstructure invariant. On the other hand, symmetries of quasiperiodic structures rely on the weaker criterion of indistinguishability[1, 2], which requires the identity of the n'th order correlation functions for all n.
We propose a method to detect the point groups of both quasiperiodic and periodic architectured materials by evaluating the criterion of indistinguishability in Fourier space.

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SIMULATION FRAMEWORK FOR THE CHEMICAL DEGRADATION IN POLYMERIC SOLIDS

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Key words: Network dynamics, Rare-event dynamics, Chemical degradation, Polystyrene

Abstract. A simulation methodology is presented that allows to examine with atomistic detail the chemical degradation in polymer glasses on macroscopically relevant time scales. Departing from simulations that are calibrated versus density-functional theory (DFT) calculations, transition-state theory and rare-event network dynamics are employed to bridge the gap to macroscopic time scales.

Chemical degradation of polymeric materials results in a deterioration of mechanical properties, which limits the serviceability of polymer products. To unravel the molecular processes at the origin of this degradation, molecular simulation can be employed. However, the timescales of chemical reactions leading to polymer degradation are typically beyond what can be reached with conventional molecular dynamics (MD) simulations. To retain molecular detail in combination with the ability to reach long timescales, so-called network dynamics has been developed [1, 2, 3, 4]. This approach focusses exclusively on local minima in the free-energy landscape and transitions between them via saddle points – with corresponding energy barriers – to describe the long-time dynamics, including chemical reactions. At the core of the network-dynamics approach is an efficient numerical procedure to – departing from local minima – establish nearby saddle-points and then in turn find other connected local minima, without the need for the full dynamics.

After discussing the main principles of this simulation strategy, initial results for the chemical degradation of polystyrene in the glassy state will be presented. For the latter, we use appropriately reparameterised reactive force-fields (ReaxFF-lg) [5] trained against density-functional theory (DFT) calculations to study the reaction pathways and energy barriers in their native glassy environment. The visited minima and saddle points along each pathway, corresponding to intermediate and transition states respectively, will eventually be used for populating the network dynamics algorithm. Our results from the large-scale-sampling of oxidation paths and their energetics in glassy configurations of polystyrene highlight how the dense, confined environment of the polymer glass crucially alters the physics of the oxidation reactions in-situ. This finding challenges the common assumption in the literature that hydroperoxide formation is the rate-determining step of performance-polymer autoxidation.

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MULTIPHYSICS MODELING OF ELECTROACTIVE POLYMERS

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Key words: Multiphysics modeling, Electromechanical coupling, Multiscale modeling

Abstract. This study introduces a multi-level homogenization framework designed to analyze the electromechanical behavior of electroactive polymer composites (EAPCs), which can transform electrical energy into mechanical motion. The framework employs a reduced mixed formulation at both the macro and micro scales, eliminating the volumetric locking and enhancing the computational efficiency. Moreover, the viscoelastic property of the elastomer matrix is incorporated, providing a thorough representation of the material's behavior.

1 INTRODUCTION

Electro-active polymers (EAPs) are an emerging class of soft active materials, which experience large deformations when they are subjected to an external electric field. EAPs are inexpensive light-weight polymeric materials, therefore, they are considered ideal candidates for high performance low cost engineering applications. A typical actuator of EAPs consist of a thin film, which is sandwiched between two flexible electrodes coating its major surfaces. Applying an electric potential difference through the thickness, causes thinning of the film and lateral expansion. For optimal design, a reliable mathematical model is needed for predicting the efficiency of the actuators, their sustainability and their safe modes of activation. Thus, several researches in the field of computational mechanics have aimed to provide such a model. Referring to the literature, several research groups have dedicated their work to profoundly study EAPs and provide efficient numerical tools [1, 2, 3]. Common EAP based actuators are made of thin films, i.e., shell like structures. Such shell-like structures have the tendency to exhibit different locking phenomena, including, shear locking, membrane locking and Poisson thickness locking. Recently, Bishara and Jabareen [4] developed a solid-shell formulation is developed adopting both the assumed natural inhomogeneous strain method ANIS and the

enhanced assumed strain method EAS. Here, the reliability of the developed solid-shell formulation is tested in capturing the large deformation of the doubly curved bi-layered spherical gripper, which may be incorporated in soft robotics, using a coarse mesh (see Fig. 1).

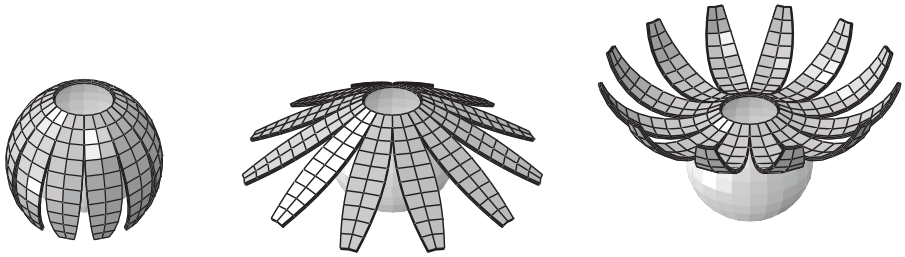

Figure 1: The deformation achieved at various time steps.

A high driving electric field is required for actuating the isotropic electric EAPs that may cause electromechanical instability and/or electric breakdown. This poor electromechanical coupling is attributed to the fact that the dielectric constant and flexibility in a polymer have an inverse relationship. Promising experimental works suggest that this limitation may be overcome by making electroactive polymer composites (EAPCs), which are flexible and have a high dielectric modulus. The aim of this research work is to provide an understanding of the mechanisms governing the electromechanical response of EAPCs undergoing large deformations. To this end, a multiphysics computational framework including the electro-mechanical coupling, thermo-electro-mechanical coupling, and the viscoelastic properties of the constituents will be presented. Furthermore, a computational homogenization that is based on the mixed finite element formulation at both the macro-scale and micro-scale (i.e. MFE^2) will be presented.

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MULTISCALE MODELING OF ELECTRO-CHEMO-MECHANICAL INTERACTIONS IN PARTICLE COMPOSITES WITH MATERIAL INTERFACES

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Key words: Multiphysics, computational homogenization, resistive interfaces

Abstract. This contribution concerns multiscale modeling of electro-chemo-mechanically coupled composites. In particular, we present a framework for computational homogenization of composite materials with material interfaces using a dual macroscopic potentials.

Computational modeling of batteries plays a pivotal role in advancing energy storage technologies by enabling the simulation and optimization of materials and processes. Batteries, particularly those based on lithium-ion and emerging technologies like solid-state systems, operate through complex electrochemical and transport phenomena coupled to the systems' mechanical properties at multiple scales. Modeling these systems involves addressing challenges such as non-linear diffusion, phase interactions, and mechanical degradation. The coupling between electrochemical processes and mechanical properties is especially critical [1], as mechanical stress can influence ion transport [2, 3] and interfacial stability, while electrochemical reactions can induce deformation and fatigue. Particle-matrix composites, commonly encountered in electrode designs, present additional complexities due to the intricate interplay between diffusion, reaction kinetics, and mechanical effects at material interfaces. Accurate homogenization techniques are essential for bridging the microstructural behavior with macroscopic performance metrics, reducing reliance on costly experimental studies or direct numerical simulations.

In this study, we investigate the computational homogenization of particle-matrix composites with material interfaces, focusing on linear transient diffusion driven by a chemical potential as a model problem. To balance computational efficiency and accuracy,

we assume micro-stationarity, enabling direct upscaling without resorting to costly time-dependent microscale simulations. As a baseline, first-order homogenization with a single macroscale chemical potential is considered; however, this approach fails to capture significant micro-transient effects accurately. To address this limitation, we propose and analyze alternative formulations employing dual macroscale potentials, one for each material phase, while maintaining stationary subscale computations.

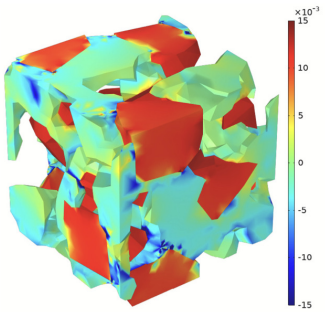

Figure 1: Simulation of the volumetric expansion ε_{vol} in a battery electrode material. [4]

Two prolongation strategies are explored: constant-linear and linear-linear. For the latter, different approaches to defining macroscale variables as inputs to the Representative Volume Element (RVE) problem are examined, including (i) averaging of the 0th and 1st gradients of the chemical potential and (ii) averaging of the 0th and 1st moments of the potential. Through a detailed numerical study, we evaluate the performance of these methods against a reference solution from Direct Numerical Simulation (DNS).

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NONLOCAL ELASTICITY VIA CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS

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Key words: Peridynamics, Nonlocal Elasticity

Abstract. Continuum-kinematics-inspired peridynamics (CPD) has been recently proposed [1, 2] as a geometrically exact formulation of peridynamics that is also variationally consistent. Unlike the original formulation of peridynamics (PD), CPD can accurately capture the Poisson effect [3]. Due to its geometrically exact nature, CPD does not suffer from zero-energy modes and displacement oscillations that have been reported in some of the state-based PD formulations. We distinguish between three types of interactions, namely, one-neighbor, two-neighbor, and three-neighbor interactions. While one-neighbor interactions recover the bond-based interactions of the original PD formalism, two- and three-neighbor interactions are inherently different to the interactions of state-based PD in that the basic elements of continuum kinematics are preserved. Through material frame indifference, we provide the appropriate set of arguments for the interactions.

Moving forward, we elaborate on thermodynamic restrictions on the interaction energies and derive thermodynamically-consistent constitutive laws through a Coleman–Noll-like procedure. Notably, we have shown that various choices for temperature or coldness satisfy the dissipation inequality and provide meaningful temperature or coldness evolution equations together with nonlocal Fourier-like conduction equations [4].

For three-dimensional elasticity, CPD builds upon three types of interactions that altogether preserve the basic notions of classical continuum kinematics, namely length, area and volume. The isotropic three-dimensional CPD formulation of non-local elasticity therefore involves three material constants, associated with length, area, and volume. Through localization and linearization, we rigorously establish relationships between the material parameters of CPD and isotropic linear elasticity. It is shown that the three material parameters of CPD reduce to two independent parameters that can be expressed in terms of any pairs of isotropic linear elasticity constants, see [5, 6] for two-and three-dimensional analysis. A remarkable finding is that CPD material parameter combinations can result in length-, area- or volume-preserving limits in that the volume-preserving limit is the familiar incompressibility bound corresponding to Poisson's ratio of 0.5 and the length-preserving limit coincides with Poisson's ratio of 0.25. In this presentation, we explain key aspects of material modeling in CPD and establish relationships between the nonlocal energy densities of CPD and the local models of classical continuum mechanics for anisotropic elasticity[7], and at large deformations.

Finally, we briefly elaborate on the aspects of numerical implementation of CPD. Several key features of CPD are demonstrated via computational examples and comparisons to the local elasticity of classical continuum mechanics using the finite element method.

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An inverse multiscale methodology for nanocomposites and its application in designing sustainable (circular) materials

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Key words: inverse methods, hierarchical multiscale modeling, homogenization, polymer nanocomposites, interphase region, in-silico materials design, biochar-polymer composites, circular nanocomposites

Abstract. Understanding and optimizing the mechanical performance of polymer nanocomposites requires characterizing the interphase—a nanoscale region between the polymer matrix and nanoparticle reinforcements. This work addresses the challenge of probing the mechanical behavior of polymer/nanofiller interphases through atomistic molecular dynamics (MD) simulations and numerical homogenization techniques. Using poly(ethylene oxide) reinforced with silica nanoparticles, we analyze the interphase by studying polymer atom density profiles, identifying thickness variations, and quantifying position-dependent mechanical properties. An inverse numerical homogenization model predicts interphase properties, showing strong agreement with MD data. Building on these methodologies, a computational framework is developed for the in-silico design and optimization of AgReCOMPOSITES—circular recycled plastic biochar products derived from agricultural and livestock waste. This framework employs hierarchical homogenization to predict mechanical properties of biochar-polymer composites, sourcing input from experimental data to optimize mixing ratios and geometrical arrangements for enhanced performance. These advances highlight the potential of multi-scale computational modeling for sustainable, circular materials design.

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THE EFFECT OF C/S RATIO ON THE ADSORPTION-DESORPTION ISOTHERMS OF C-S-H

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Key words: Molecular simulations, Adsorption-Desorption, Drying, Hysteresis

Abstract. Water plays a key role in the durability of cement-based materials, particularly within the nanopores of the calcium silicate hydrate gel (C-S-H), which is the main contributor to the strength of the concrete. However, the chemical stoichiometry of C-S-H is variable and depends on the calcium-to-silicon (C/S) ratio, which influences its interaction with water. In this study, we generated C-S-H structures with varying C/S ratios and investigated the water adsorption-desorption isotherms using the Grand Canonical Monte Carlo (GCMC) method at ambient temperature. The results demonstrate that the C/S ratio significantly affects the adsorption-desorption behavior of water: an increase in the C/S ratio leads to a higher water content. Furthermore, the desorption branch closely follows the adsorption path, indicating limited hysteresis. These findings provide insight into the nanoscale water dynamics in C-S-H, with potential implications for improving the durability and performance of cement-based materials.

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GRADIENT-EXTENDED MODELING OF POROUS MEDIA ACROSS THE SCALES

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Key words: Porous media, gradient-extended models, multiscale methods

Abstract. The inherent heterogeneity of porous media leads to distinct physical responses at different length scales. For example, the microscopic scale of a porous medium is characterized by a solid skeleton that is permeated by a pore network. In a fluid-saturated porous medium, the pore network is entirely filled with fluid, which could flow through the pore space. The resistance to flow depends on several conditions; for example, it increases with increasing viscosity of the fluid and it decreases with increasing size of the pores. The observable flux of a fluid through a porous medium at larger length scales is the result of physical interactions at the lower scales and is thus strongly related with its microscopic properties and its microstructure. Associated phenomenological continuum models are typically based on the celebrated Darcy law of fluid flow through porous media.

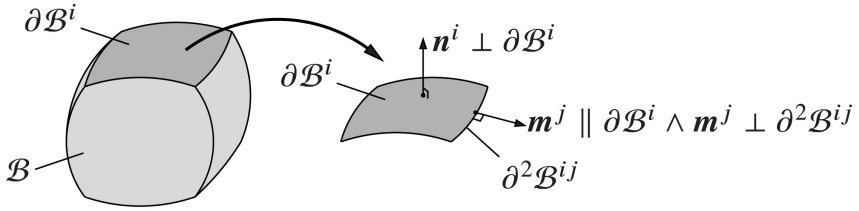

Figure 1: Continuum-mechanical view on a porous medium in a gradient-extended modeling framework (illustration inspired by the mechanical version due to Javili, dell'Isola and Steinmann [3].

In the present talk, we take a closer look at the modeling of fluid flow through porous media *at* and *across* different length scales, all of which are assumed to be sufficiently large such that Darcy's law or extensions thereof can still be applied. Our goal is to shed some light on the size-dependent physical behavior of porous media. To achieve this,

we will introduce different higher-order continuum models and discuss their numerical implementations within phenomenological and multi-scale scenarios.

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GENERATIVE DIC-FEMU WITH UNKONWN FIELDS OF MATERIAL CONSTANTS ENABLED BY SPARSE GAUSSIAN PROCESS PRIORS.

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Key words: FEMU, DIC, SPDE, Gaussian Processes, Bayesian inverse problems

Abstract. In this contribution, we will develop a methodology to identify fields of unknown material constants given DIC measurements. The FEMU-DIC method is made Bayesian, leveraging the computational tractability of SPDE-based Gaussian Processes to deliver interpretetable statistical parameters that may be used to predict the distribution of stiffness of future components.

Calibration of model parameters based on full-field measurements is now very commonly employed in mechanical and material engineering practices. This may be done in different ways, for instance by using advanced frameworks such as the Virtual Field Method, or Integrated Digital Image Correlation (I-DIC) [1]. In the present paper, we concentrate on a classical paradigm where full displacement fields are recovered using standard DIC algorithms, and model parameters are subsequently identified using FEMU by minimising an appropriately crafted measure of the difference between the simulated displacement fields and that obtained by DIC. Usually, the model parameters to be identified are constant across the specimen. However, in this study, we aim to account for macroscopically observable variations in material properties and seek to determine material parameters in the form of unknown spatial fields.

This introduces several challenges, amongst which (i) appropriately discretising the field of unknown parameters, (ii) computing the gradient of the inverse problem cost function with respect to an arbitrary large number of discrete parameters and (iii) using a carefully-crafted regularisation methodology to adress the issue of non-unicity of continuous unkown fields. Points (i) and (ii) will be addressed by means of finite element discretisations and

adjoints-based methodologies, respectively, the second point being made very efficient using the automatic differentiation capabilities of the FEniCS software. For the third point, we will rely on a stochastic-PDE-based regularisation technique. This may be viewed as using a Matérn Gaussian Process prior in a Bayesian inverse problem setting, with the distinct advantage over standard, Kernel-based Gaussian Process priors that only sparse operator inversions are required.

We will demonstrate that the approach efficiently delivers correct fields of material constants when associated with algorithms to automatically adjust the regularisation hyperparameters in an empirical Bayes fashion.

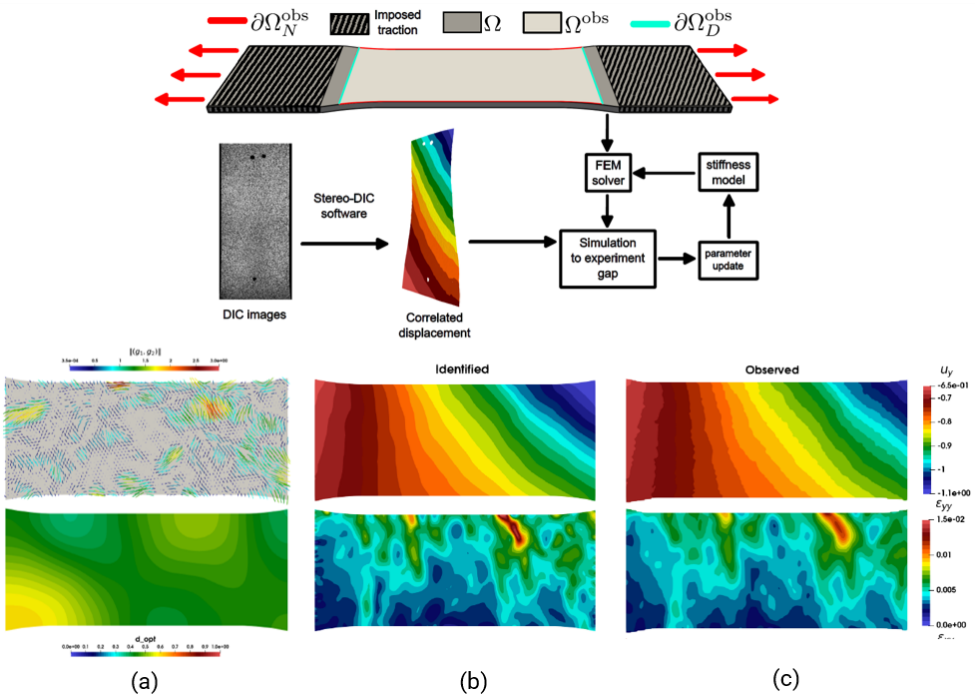

Figure 1: DIC-FEMU setup (top) and result of the inverse problem (a-c)

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COMPUTATIONAL MODELING OF INTERTWINED ARCHITECTED MATERIALS

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Key words: Woven Network, Architected Material, Contact Modeling, Homogenization

Abstract. Intertwined, woven, and notted networks are classically found in textiles and have more recently also attracted attention for the creation of architected materials with as-designed properties. The relative motion between fibers in the network, involving contact and friction between structural elements, endows such structures with unique properties, which derive from the complex structural interactions and which depend on the structural topology, the base material properties, and the frictional properties. Modeling such structures is challenging and the focus of this contribution. We present an efficient computational framework that leverages a beam-based representation of the fiber network: at the fiber level we use a nonlinear corotational kinematic description and elastic-plastic-damage constitutive models of the base material; at the structural level, a variational beam contact formulation accounts for finite sliding. This setup is applied to a suite of benchmarks, which verify the accuracy in comparison with 3D finite element simulations and experiments. Finally, a design approach allows us to perform structural optimization.

We focus on woven lattices that are constructed by interlacing fibers or struts in a regular pattern, providing a uniform and predictable structure ideal for applications requiring consistent mechanical behavior (see Figure 1). This is distinct from classically used knotted structures, which are formed by irregularly tying fibers, creating complex, nonlinear responses with localized points of stiffness and flexibility. Accurately simulating the mechanics of fabrics and knots requires a fast, high-fidelity model that captures (i) the complex frictional contact interactions between the slender fibers and (ii) the involved geometrical and material nonlinearities at the fiber level.

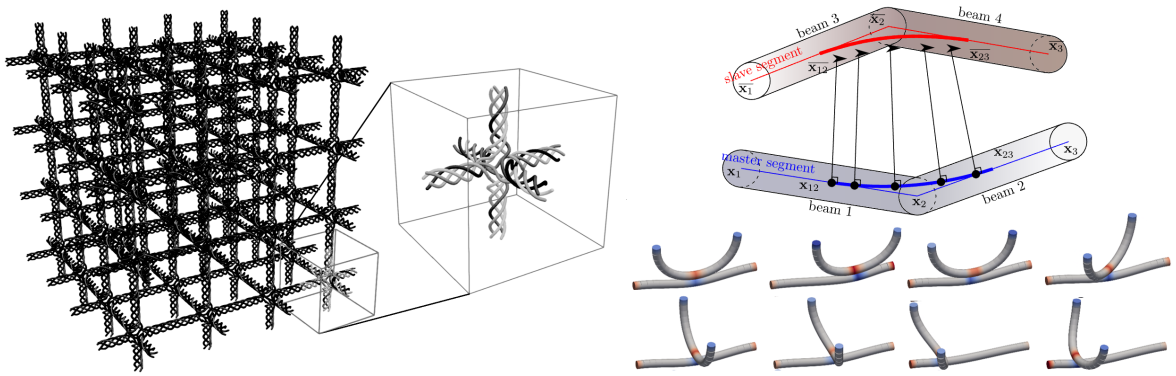

Figure 1: Modeling of intertwined architected materials: shown on the left is an example structure composed of periodically repeating intertwined fibers; shown on the right is a schematic of the conforming model for frictional contact along with a simulated example of sliding fibers.

To address challenge (i), we make use of a conforming approach [2], which discretizes each contact element with a given number of quadrature points, for each of which a one-sided orthogonal problem is solved, whose solution is always unique (see Figure 1). This avoids the complications of frequently used pointwise contact models, which are well-established but become problematic in the context of distributed contact models that accurately incorporate friction. To tackle challenge (ii), we use a corotational beam description for slender rods, combined with a variational, inelastic 1D base material model [1]. The 1D model is integrated in the corotational beam framework by discretizing the cross section with multiple quadrature points and assigning to each of those independent internal variables accounting for plasticity and damage. The material and friction models have been calibrated experimentally for 3D-printed polymers, which are also used in fabrication and characterization experiments of the proposed intertwined architected materials. In this contribution, we will discuss the theoretical model, computational framework, and especially the application to intertwined architected materials, which offer new, untapped property and design spaces.

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METAMATERIALS FOR ACOUSTIC AND ELASTIC SUBWAVELENGTH APPLICATIONS: DESIGN AND MULTI-SCALE MODELLING

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Key words: Metamaterials, Local Resonance, Computational Homogenization

Abstract. This talk will present the recent advancements in the computational homogenization techniques for modelling elastic and acoustic wave propagation in locally resonant metamaterials.

The past two decades have been marked by the ever increased interest into the development of various types of metamaterials, i.e. architected materials exhibiting properties beyond those achievable through chemistry and microstructure. A class of metamaterials designed to manipulate the propagation of elastic/acoustic waves is of particular interest here as it opens unprecedented possibilities for a broad class of applications ranging from noise/vibration insulation, to acoustic cloaking, acoustic lenses going beyond the diffraction limits, seismic isolation, tunable waveguides, adaptive passive vibration control, acoustic diodes, and many more. Various physical principles are being harnessed for obtaining metamaterials' extraordinary properties. This work focuses on metamaterials based on one of these principles, i.e. the localized resonance, which is of a particular interest for subwavelength applications, i.e. when the wavelength being manipulated is (significantly) larger compared to the size of the metamaterial units.

In this talk, first several examples of locally resonant subwavelength metamaterials will be given, followed by a recently proposed design of a locally resonant metasurface the realises the enhanced reflection at a negative reflection angle [1].

Next, the need for modelling techniques that allow the analysis and design of subwavelength metamaterial domains of finite sizes, complex geometries and non-trivial, non-harmonic loadings, possibly involving non-linearities will be discussed. As a good candidate, transient computational homogenization methodology will be presented. The approach is applicable to general non-linear problems, while in the linear elastic case it was

shown to provide the closed-form homogenized effective constitutive relations. In this talk, the extension of computational homogenization methodology to fluid flow through porous structure, including local resonances, will be presented and its application to acoustic metamaterials will be illustrated [2, 3]. Finally, computational homogenization for locally resonant metamaterials including general, non-classical damping, will be addressed.

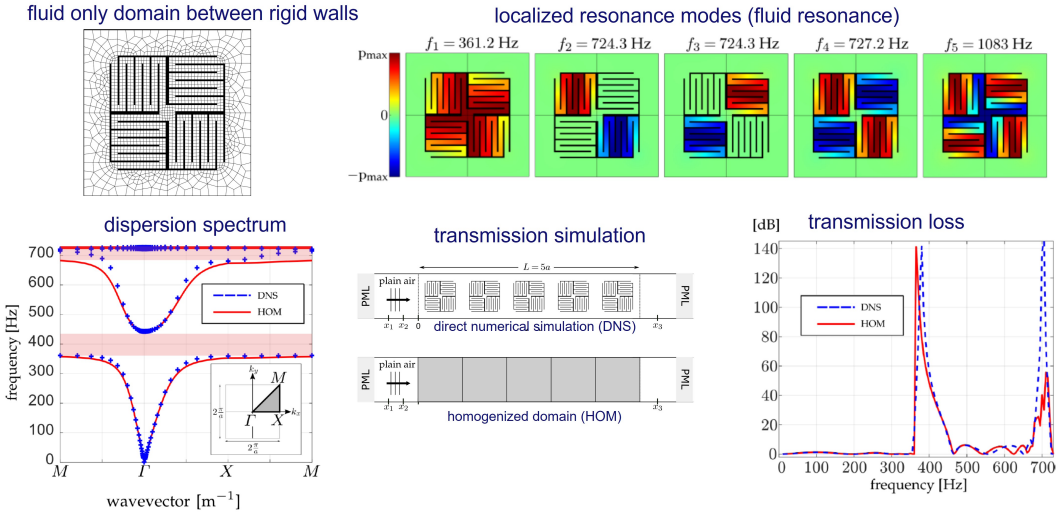

Figure 1: Computational homogenization of a labyrinthine acoustic metamaterial [3].

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ENHANCING EPOXY POLYMER NETWORK SIMULATIONS IN LAMMPS: A COMPARATIVE STUDY OF CROSSLINKING ALGORITHMS AND TOPOLOGICAL UPDATES

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Key words: Bio-sourced epoxy, molecular dynamic, crosslinking

Abstract.

In this study, we focus on generating and analyzing the polymer network topology of epoxy resins, specifically DGEBA and DETDA molecules, using two crosslinking approaches within the LAMMPS simulation software. The first method utilizes the REACTER approach to simulate the curing process, while the second approach employs a modified version of the bond/create to ensure the topology of molecules is dynamically updated after bond formation. This modification enhances the precision and reliability of the simulated network structures. Both methodologies are evaluated to compare their effectiveness in capturing the network formation process, with an emphasis on their suitability for characterizing microstructure-property relationships and mechanical behavior. The results provide insights into the advantages and limitations of each approach for simulating crosslinked polymer systems, with potential implications for the design of high performance bio-sourced epoxy materials.

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COMPUTATIONAL HOMOGENIZATION OF POROUS MEDIA – APPLICATION TO ION TRANSPORT IN BATTERIES

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Key words: Computational homogenization, Porous media, Transport

Abstract. This contribution concerns computational homogenization of porous media. In particular, we discuss procedures for predicting deformation dependent transport properties for battery applications.

Understanding and modeling the response of porous media, i.e., microheterogeneous materials consisting of a solid skeleton and fluid filled pores, is important for many applications in science and engineering. One emerging technology is the so-called structural battery, which is a composite material able to store (electro-)chemical energy while being part of the load baring structure. One version of the structural battery being developed utilizes a so-called Structural Battery Electrolyte (SBE), which consists of two phases: a solid phase (a porous polymer network) and a liquid electrolyte that serves as the carrier of ions, most importantly Li-ions. Under mechanical load, the ion transport is brought about by migration (from the electric field), diffusion (driven by the gradient of the chemical potential), and - under the influence of mechanical load - convection from fluid motion (seepage). These couplings have been considered at the cell level by Carlstedt et al. [1]. However, influence of mechanical loads on the mobility (pertinent to migration and diffusion) and permeability (pertinent to convection) have not been studied for theses systems.

Motivated by, but not limited to, the study of SBE in structural batteries, we revisit computational homogenization of porous media, see e.g. [2]. In particular, we study different simplifications to study a hierarchy of models. First, we consider a linearized model

and discuss the procedure for determining the linear relations at the macro-scale pertinent to Biot theory. Secondly, in order to upscale deformation dependent mobilities and permeabilities, we adopt a finite deformation framework to assess the decoupled (drained) deformation and transport under large deformation of the porous media. Finally, we discuss how to adopt the developed models in effective macro-scale computations.

Numerical example simulations are performed on synthetic Representative Volume Elements (RVEs) mimicking different design proposals for SBE, cf. [3]. For different assumptions on the (fairly) basic model assumptions at the pore scale, we quantify the effective properties at the macroscale from statistical sampling of microstructure geometries. As an example, Fig. 1 illustrates how the fluid seepage brought on by a pore pressure gradient reduces under compressive loading.

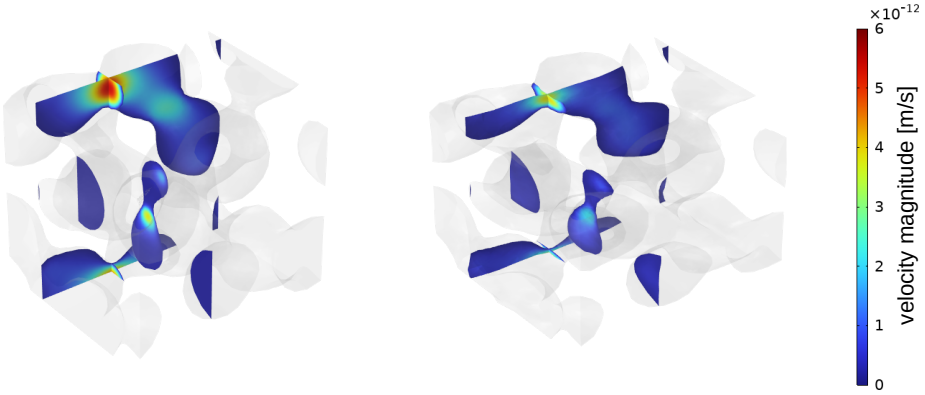

Figure 1: Simulation of seepage in a porous media for undefomed (left) and deformed (right) pore space.

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NONLINEAR TWO-SCALE BEAM SIMULATIONS ACCELERATED BY THERMODYNAMICS-INFORMED NEURAL NETWORKS

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Key words: Neural Network, Hyperelasticity, Architected Material, FE^2, Beam

Abstract. Beam-based architected materials can be subjected to large strains in a range of applications. Finding efficient and accurate models for these materials at finite strains is a challenging task as their microstructures consist of many individual slender beam members that exhibit nonlinear effects due to their geometry (large rotations) and behavior (e.g., hyperelastic materials). Therefore, there is a need for an efficient modeling approach capable of accurately capturing the physics of these large, complex systems.

Following a formal asymptotic dimension reduction approach, we decompose the problem into an efficient macroscale simulation of the beam's centerline and a finite elasticity problem on the cross-section (microscale) at each point along the beam. From the solution on the microscale, an effective energy is passed to the macroscale simulation, where it serves as the material model. However, this two-scale approach comes at a high computational cost. To leverage the efficiency of the macroscale beam simulation, we therefore introduce a Sobolev-trained thermodynamics-informed neural network, which serves as a surrogate model for the costly microscale simulations, whose effectiveness we demonstrate in a suite of examples, ranging from cantilever beams to 3D beam networks [1].

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Phase field modeling and FEM simulation of bone fracture occurring in human vertebra after screws fixation procedure

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Key words: Phase field approach to fracture; Finite Element Method.

Abstract. Metallic pedicle screws are used in spine fusion procedures when the intervertebral discs are damaged by aging or trauma. Spinal fusion joins two or more diseased vertebrae, preventing motion at the vertebral segment. Understanding the stability in the lumbar spine of a human vertebra after screw fixation and the possibility of fracture is still a critical unsolved clinical problem. In the present work, the effect of pedicle screws angulation (medial and cranio-caudal) and physiological loading of the implant (i.e., flexion, extension, axial rotation) are investigated on a patient-specific model of a lumbar vertebra (L4), derived from clinical CT images, see Fig.1. The bone has been modeled as brittle material with inhomogeneous properties fine-tuned on biomedical CT-scan data accounting for its cortical and trabecular domains [1]. The phase-field approach [2], based on a variational approach to damage localization, is particularly suited to describe crack nucleation and complex fracture patterns occurring in bone and porous materials. A finite element algorithm, based on the spectral decomposition of the strain energy density, has been developed in the software FEniCS. The proposed phase field framework can help to elucidate

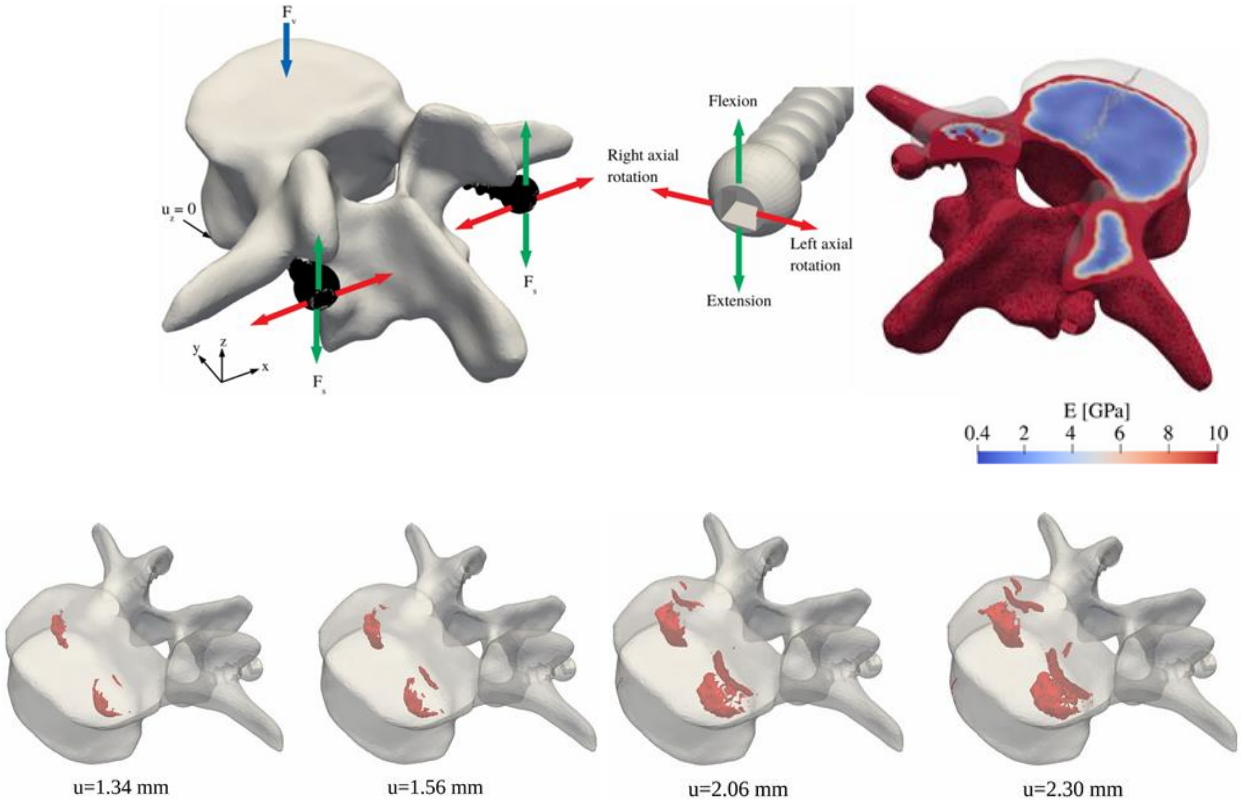

Figure 1: Boundary loading conditions; Young modulus distribution; Phase field evolution.

scenarios where different damage patterns, such as crack nucleation sites and crack trajectories, play a role after the spine fusion procedure. Overall, the phase field results can potentially shed more light on microstructure bone features not directly available to the medical community. Finally, it will help enhance clinical interventions and reduce post-surgery bone failure and screw loosening.

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TAILORED GAUSSIAN PROCESS MODELING FOR POLYCRYSTALLINE TEXTURE REPRESENTATION

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Key words: Microstructure, Texture, Pole Figures, Gaussian Process Regression

Abstract. A tailored Gaussian Process Regression (GPR) [1] model is proposed for the reconstruction of pole density functions in texture analysis [2]. This approach incorporates spherical-periodic distance measures into conventional stationary kernels to effectively capture localized texture features. A key innovation is the introduction of a log-linear data transformation that ensures non-negativity of both interpolated function values and stochastic intervals, leading to physically consistent reconstructions. The proposed approach is systematically evaluated on synthetic texture datasets, examining the influence of distance measures, kernel selection, and hyperparameter optimization. Moreover, comparisons with the conventional spherical harmonics method will be presented during the conference.

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THE MAGNETO-MECHANICAL RESPONSE OF MECHANICALLY-SOFT HARD MAGNETORHEOLOGICAL ELASTOMER FOAMS

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Key words: Magnetorheological elastomer, Porous materials, Magnetorheological foams, Magneto-mechanical response

Abstract. Hard magnetorheological elastomers (h-MREs) are two-phase composite materials comprising micron-scale particles with significant remanent magnetization properties that are embedded in a soft elastomer matrix. In this work, we extend our work to h-MRE foams with soft mechanical response (Young's modulus in the order of 100 kPa). In this study, we analyze the magneto-mechanical behavior of h-MRE foams by combined modeling and experimental testing. In particular, we study the change of the magnetic field surrounding the h-MRE foams under compressive mechanical loads. A qualitative continuum modeling of the h-MRE foam guides a set of experimental tests, which allows in-turn to calibrate the model parameters. Additional numerical simulations permit to probe further the response of such foams under non-trivial loading conditions and design potential sensing devices by exploiting the surrounding magnetic changes. This study allows for a better understanding of h-MRE foams, providing fundamental insights for their future applications like soft force sensors.

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Molecular Dynamics prediction of 3D dislocation density in Aluminium

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Key words: Molecular Dynamics, Dislocation Density

Abstract. Accurate prediction of the mechanical behavior of commercial aluminum alloys requires incorporating the influence of microstructural features, such as dislocation density, into macroscopic constitutive models. While experimental techniques provide valuable insights, direct observation of dislocation dynamics at the atomistic scale remains challenging. This study employs advanced molecular dynamics (MD) simulations to investigate the evolution of dislocation density in representative microstructures of commercial aluminum alloys subjected to various loading conditions. This multiscale approach bridges the gap between atomistic and continuum scales, providing a deeper understanding of the underlying mechanisms governing the mechanical response of aluminum alloys.

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CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS FOR TRANSVERSE ISOTROPY

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Key words: Peridynamics, Anisotropy

Abstract. Accounting for the combined effects of mechanical anisotropy and nonlocality is critical for capturing a wide range of complex material behaviour, especially at small length scales. Such directional dependence is present in many biological and engineered materials to achieve optimal performance. While the local (Cauchy) continuum theory for transversely isotropic materials undergoing finite deformations is well understood, this is not the case for the nonlocal continuum theory of peridynamics (PD) proposed by Silling [1]. Continuum-kinematics-inspired peridynamics (CPD) [2], a strongly non-local continuum formulation, provides the essential underpinning theoretical and numerical framework to realise this objective.

The formalism of rational mechanics is employed here to rigorously extend CPD to the important case of transverse isotropy at finite deformations while retaining the fundamental deformation measures of length, area and volume intrinsic to classical continuum mechanics [3]. Details of the anisotropic contribution to the potential energy density due

to length, area and volume elements are given. A series of numerical examples serve to elucidate the theory presented, see Figure 1.

Furthermore, recent developments to mitigate the computational overhead associated with the requirement to compute multiple nested integrals at each collocation point in CPD are presented.

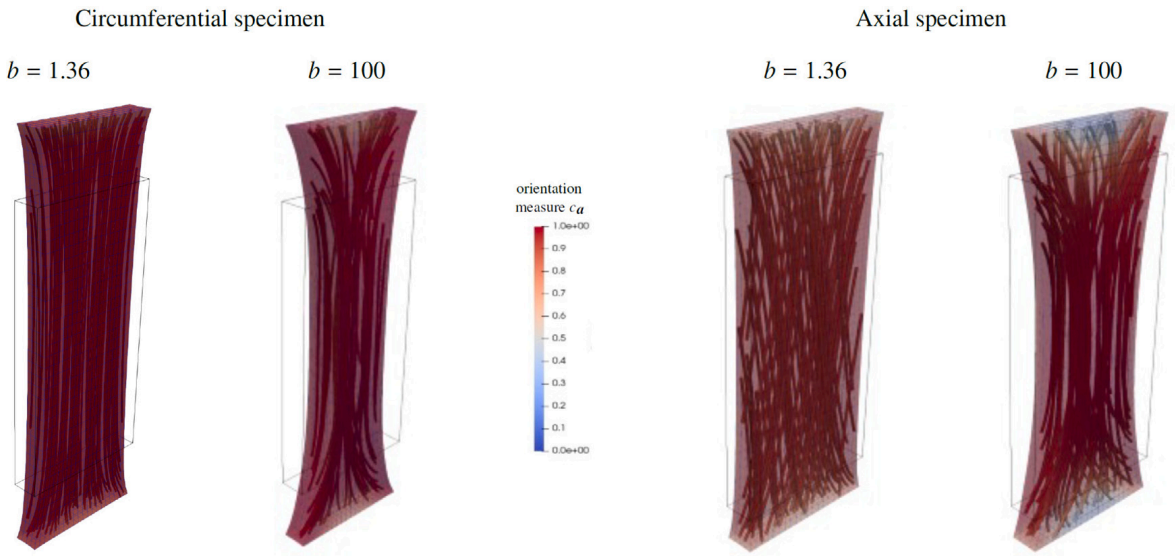

Figure 1: CPD prediction of the current (mean) collagen orientations. Results are shown for circumferential and axial specimens. The cases on the left correspond to dispersion in the collagen fibres, and on the right to no dispersion (fully aligned fibres.

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MODELING OF ADDITIVE MANUFACTURING PROCESSES OF METALS – A MUSLTISCALE APPROACH

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Key words: Laser Powder Bed Fusion, phase transformation, microstructure, homogenisation, relaxation

Abstract. This work presents a multiscale modelling approach for laser powder bed fusion processes, focusing on thermomechanically coupled material response and an efficient simulation framework. Phase transformations are explicitly taken into account to predict microstructure evolution, residual stresses, and deformation, respectively distortion.

An efficient mutliscale modelling framework (without full scale separation) for Powder Bed Fusion-Laser Beam / Metals (PBF-LB/M) is proposed, cf. [1]. The model describes the respective material states – powder, melt and solid – while incorporating phase transitions between these; see Fig. 1(left) and Fig. 2(a). Physical phenomena, such as transformation-induced strains together with mass conservation, are included to naturally capture layer thickness reductions during phase transitions. For the scan island, a simplified material model is used to extract micromechanically motivated inherent strains $\boldsymbol{\varepsilon}^{\mathrm{inh}}$; see Fig. 1(middle). These strains enable efficient simulation-based prediction of residual stresses and resulting deformation in the final part, see Fig. 1(right) and Fig. 2(b), distinguishing this method from empirical averaging approaches.

The framework also supports the incorporation of more advanced solid-state phase transformation models tailored for multiphase alloys, such as Ti_6Al_4V, as introduced in [2]. Unlike empirical approaches, such as Johnson-Mehl-Avrami-Kolmogorov models or Koistinen-Marburger models, the proposed framework relies on related energy densities and physics-based evolution equations. To be specific, phase evolution is governed by dissipation functions, with coefficients determined by parameter identification using (limited)

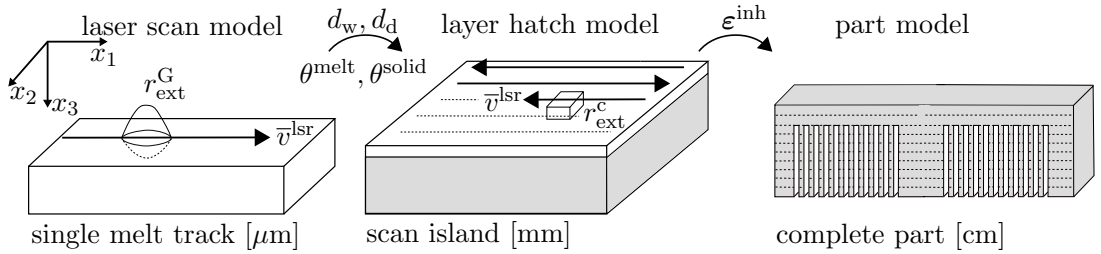
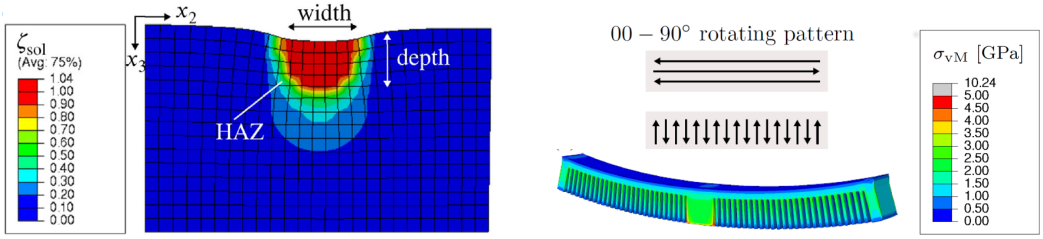


Figure 1: Illustration of the three different levels (with respective dimension) considered in the multiscale approach, where the melt pool dimensions d_w, d_d, temperatures θ_{melt}, θ_{solid} and the inherent strain $\boldsymbol{\varepsilon}^{inh}$ are passed from one level to the other. White structures are initially made of powder, grey body consists of solid material. Reproduced from [1] under the terms of the Creative Commons Attribution License (CC BY 4.0).



(a) (b)

Figure 2: Process simulation results with multiscale approach: (a) single melt track – Gaussian heat source and phase transformation model to determine phase fraction ζ_{sol} of re-solidified material; (b) complete part – time-efficient purely mechanical simulation to predict residual stresses σ_{vM} (von Mises equivalent stress) and distortion. Reproduced from [1] under the terms of the Creative Commons Attribution License (CC BY 4.0).

experimental data or Continuous Cooling Transformation (CCT) diagrams. This enables accurate numerical reproduction of CCT diagrams and reliable predictions of microstructure evolution, strains, and stresses. The flexibility of the model allows for extensions to additional phases and materials, making it a versatile and robust tool for the simulation of additive manufacturing processes.

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A better synergy between meshing and computing to track fronts (and more): X-MESH

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Key words: eXtreme mesh deformation, X-FEM, configurational mechanics, variational r-adaptation

Abstract.

In current simulations, the level of interaction between the mesh and the computation is fairly low. A mesh is created upstream on a mainly geometric basis (respecting an external surface and respecting the aesthetics deemed necessary for the mesh). Specific refinements are sometimes required, as in the case of crack faces or boundary layers in flows. Sometimes the initial mesh is adapted based on an error map estimated a posteriori, or the mesh is changed because it has become too distorted, as is the case in ALE simulations where the relative size of elements on either side of an interface can become enormous. Another reason for modifying the mesh occurs in large-transformation calculations where, if nothing is done, some finite elements may flip over during the simulation.

Modifying the mesh during a calculation generally involves stopping the calculation abruptly, with a necessary projection of the fields between the old and new meshes. This operation has a detrimental effect on solution quality and computation time.

In this presentation, we look at a new way of tracking fronts. The idea is to allow nodes to leave the front or join the front. In this way, nodes can simply move into their immediate vicinity to relay the front. The front, on the other hand, migrates through the mesh possibly over long distances and can undergo topological transformations, which is not the case in the ALE approach. A first paper deals with the propagation of solidification fronts [1], followed by a second for the tracking of material fronts such as interfaces between immiscible fluids [2]. Finally, a third paper deals with front propagation in the so-called porous medium

equation which is a one-phase problem [3].

The X-MESH front tracking generally leads to very flattened or even zero-size elements, and therefore to an eXtreme mesh. Hence the name X-MESH. Surprisingly, the presence of very flattened elements can be managed quite easily within the finite element framework. This is what we have achieved in paper [4], which introduces the tempered finite element method (TFEM for Tempered FEM).

The X-MESH approach also takes an interesting turn in fracture mechanics. Elements in the crack path naturally flatten out to generate a displacement jump. Progress in this direction will be presented.

In addition to front tracking, the presentation will also look at optimal mesh design in the variational sense. We will discuss an ideal synergy between meshing and computing, both for the front and for the bulk phases on either side.

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HIERARCHICAL BIAXIAL CURVATURE IN HYGROMORPHIC BILAYERS: A MODEL FOR PINE CONE DEFORMATION AND 4D-PRINTED MATERIALS

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Key words: Hygroelasticity, 4D printed materials, Hygromorph

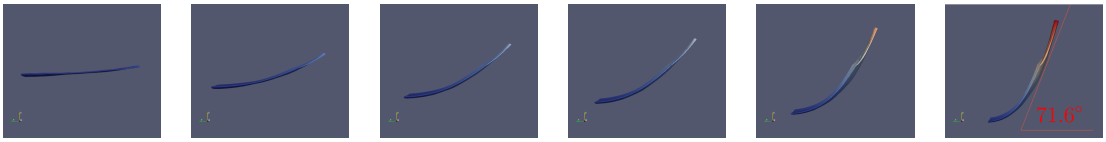
Abstract.

Natural bilayer structures, such as pine cone scales, exhibit hierarchical deformation in response to environmental humidity changes, a key mechanism for designing 4D printed hygromorphic materials. We present a generalized analytical model for predicting complex shape-morphing in hygroscopic bilayers, addressing limitations in existing approaches that oversimplify anisotropic material behavior [1]. By extending Föppl-Von Kármán plate theory to incorporate both anisotropic hygroscopic expansion coefficients and spatially varying humidity fields, we establish a unified framework for biaxial curvature prediction.

Numerical simulations via FEniCS finite element modeling validate the theoretical framework when applied to pine cone scale systems. The model resolves a hierarchical curvature regime transition−longitudinal to transverse dominance−modulated by material anisotropy, geometric scaling, and hygroscopic gradients, demonstrating quantitative alignment with biological deformation mechanics [2].

This mechanistic insight advances the design for 4D printed programmable materials, enabling humidity-driven morphing control with applications in soft robotics, adaptive

architecture, and bio-inspired actuators.



(a) RH=30 (b) RH=40 (c) RH=50 (d) RH=60 (e) RH=70 (f) RH=80

Figure 1: Hierarchical deformation of pine cone scales under changing Relative Humidity (RH): from longitudinal curvature dominance to transversal curvature dominance.

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FULLY COUPLED MODEL FOR ANALYSIS OF SHAPE MEMORY ALLOY

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Key words: Shape Memory Alloy, Phase-field Model, Fully Coupling

Abstract. A formulation of the fundamental principles of the shape memory alloy (SMA) is presented. The formulation uses the thermomechanical theory considering phase-field energy that characterizes its unique functionality of SMA.

This material introduces the formulation of a shape memory alloy (SMA), covering the fundamental principles that dictate its behavior, such as thermo-mechanical properties and phase transformation mechanisms that define its distinctive functionality. The formulation is based on phase-field energy. The equations for the SMA are as follows:

Equilibrium: $\sigma_{ji,i} + b_i = 0$ (1)

Kinematics: $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ (2)

Hooke's law: $\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \varepsilon^0{}_{kl})$ (3)

Phase-field kinetic law [1]:

$$\frac{\partial \phi^{\mathrm{m}}}{\partial t} = L[-\Delta f(A\phi^{\mathrm{m}} - B\phi^{\mathrm{m}2} + C\phi^{\mathrm{m}}\sum_{\mathrm{m}=1}^{\mathrm{n}}\phi^{\mathrm{m}2}) + a^2\nabla^2\phi^{\mathrm{m}} + \varepsilon^{\mathrm{m}}{}_{ij}C_{ijkl}(\varepsilon_{kl} - \varepsilon^0{}_{kl})] \quad (4)$$

where σ_{ij} is the Cauchy stress, b_i is the body force, ε_{ij} is the linear strain, u_i is the displacement, C_{ijkl} is the elastic constant matrix, $\varepsilon^0{}_{ij}$ is the eigenstrain, ϕ^{m} is the order variable of variant m, ε^{m} is the eigenstrain of variant m, L is the mobility, Δf is the constant expressing the energy difference between phases, A, B, C are the constants, and a is the diffusion constant.

The boundary definition is as follows:

$$\sigma_{ji} n_j = \overset{(n)}{t}_i \tag{5}$$

The free energy of the equations are as follows:

$$\psi = \frac{1}{2}(\varepsilon_{ij} - \varepsilon^0{}_{ij}) C_{ijkl} (\varepsilon_{kl} - \varepsilon^0{}_{kl}) \qquad \text{Elastic energy}$$

$$= \frac{1}{2}\sum_{m=1}^{n} a^2 \phi^m{}_{,i} \phi^m{}_{,i} \qquad \text{Gradient energy}$$

$$= \psi_{chem}(\phi^1, \phi^2, \cdots \phi^n) \qquad \text{Chemical energy}$$

Based on the equation, we have the constitutive laws of conjugate quantities, σ_{ij}, η^m and ξ^m, for ε_{ij}, ϕ^m and $\phi^m{}_{,i}$ respectively:

$$\sigma_{ij} = \frac{\partial \psi}{\partial \varepsilon_{ij}} = C_{ijkl}(\varepsilon_{kl} - \varepsilon^0{}_{kl}) \tag{6}$$

$$\eta^m = \frac{\partial \psi}{\partial \phi^m} = -C_{ijkl}(\varepsilon_{kl} - \varepsilon^0{}_{kl}) \frac{\partial \varepsilon^0{}_{ij}}{\partial \phi^m} + \frac{\partial \psi_{chem}}{\partial \phi^m} \tag{7}$$

$$\xi^m = \frac{\partial \psi}{\partial \phi^m{}_{,i}} = a^2 \phi^m{}_{,i} \tag{8}$$

Here, the balance equation of the micro-force and the boundary definition are the follows [2]:

$$\xi^m{}_{i,i} + \pi^m + \gamma^m = 0 \tag{9}$$

$$\xi^m{}_i n_i = \overset{(n)}{\lambda}{}^m \tag{10}$$

where π^m is the internal micro-force, γ^m is the external micro-force which usually becomes zero, and $\overset{(n)}{\lambda}{}^m$ is the surface micro-force which usually also becomes zero, too [3]. (An explanation of what the micro-force in phase transformation in SMA is should be written here.) From thermodynamic arguments about π^m, we have the following constitutive relationship of π^m [2]:

$$\pi^m = -\eta^m - \frac{1}{L}\frac{\partial \phi^m}{\partial t} \tag{11}$$

Substituting the constitutive relationship of πm into the micro balance equation, we obtain the following transient phase-field equation:

$$\frac{\partial \phi^m}{\partial t} = L[\xi^\mu{}_{i,i} - \eta^m + \pi^m] \tag{12}$$

The results with the numerical analyses in the staggered scheme and monolithic scheme are compared.

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COMPARISON OF MULTISCALE METHODS FOR MODELING PERFORATED PLATE IN COMPUTATIONAL STRUCTURAL MECHANICS

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Key words: Multi-scale methods, perforated plate, computational homogenization, Transformation Field Analysis (TFA), Mori-Tanaka, Hybrid-Trefftz.

Abstract.

Riveted assembly areas play a crucial role in the resistance of mechanical structures subjected to shocks and impacts, particularly in the aeronautical sector. A numerical simulation analysis of the generated physical phenomena necessitates precise modeling of both the entire structure and the assembly zone. Despite advancements in computing power, simulations of this nature remain complex due to the need for highly refined modeling in assembly areas, which generates a stable time step that is often incompatible with the numerical simulation of an aeronautical structure. To address this challenge, an approach based on modeling assembly zones using plate hybrid-Trefftz displacement (HT-D) elements was therefore considered. Such elements have demonstrated significant effectiveness in the linear elastic domain only. Consequently, this research aims to develop an analogous approach to address materially and geometrically non-linear problems. Different multi-scale methods (such as Transformation Field Analysis - TFA), model reduction (Proper Orthogonal Decomposition) or machine learning (Neural Wetworks) are therefore considered to meet this need. The TFA approach is firstly considered for its capability to localize fields. However, a limitation of the TFA method is that it relies on a very fine discretization of the Representative Elementary Volume (REV) to obtain reliable results, which leads to a rapid increase in computational costs. To overcome this issue, a mixed approach combining the TFA method with the Mori-Tanaka theory is proposed. Some preliminary results indicate that the Mori-Tanaka method can significantly reduce the computational costs while maintaining the accuracy when compared to the TFA approach. The purpose of this poster is to evaluate the effectiveness of the proposed method in comparison to existing methods (HT-D and TFA methods).

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AN FFT-BASED METHOD FOR COMPUTING THE THERMAL, HYDRAULIC AND MECHANICAL RESPONSE OF COMPOSITES

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Keywords: FFT-based homogenization, Multiphysics

Abstract. Fast Fourier Transform (FFT) methods have been widely used for more than a decade as an alternative to more conventional numerical techniques (FEM, BEM). These methods allow estimating the elastic mechanical response of composite materials, by means of the discretization of the Lippmann-Schwinger equation, and the truncation of the Fourier series values. The basic scheme, a fixed-point algorithm of easy application, is limited when multiphase systems with both pores and infinitely rigid inclusions are used. Using the approach proposed by Sab et al. [1][1], we present the mathematical analysis of three different FFT-based numerical schemes for homogenization of composite media in the framework of : (i) linear plasticity, evaluating the plastic evolution with von Mises, Drucker-Prager and Cam clay yield criteria, (ii) hydraulic field, calculating the isotropic permeability tensor, K_{hom}, from the Darcy/Darcy problem, and (iii) thermal field, where the isotropic thermal conductivity tensor, λ_{hom}, is formulated for Fourier to Fourier upscaling. The accuracy of each scheme is evaluated by comparisons with a finite element solver and analytical solutions for simple microstructures.

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ON EFFICIENCY AND ACCURACY OF EIGENSTRAIN HOMOGENIZATION METHOD FOR MODELING POLYCRYSTALLINE MATERIALS

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Key words: Reduced order modeling, Nonlinear homogenization

Abstract.

Crystal plasticity finite element (CPFE) and spectral methods are commonly employed to simulate and characterize the viscoplastic response of metals and alloys at the microstructural scale. These direct methods remain computationally expensive for the characterization of single scale problems with complex microstructural features. Furthermore, they are infeasible for multiscale analyses of large scale engineering structures that tightly couple them to a structural analysis. The need for higher computational efficiency in this regard motivates the development of reduced order modeling (ROM) strategies. Computational ROMs typically consist of an offline model training stage, where the ROM is constructed based on prior simulations, and a model execution (online) stage, where the solution is searched over a coarse approximation space spanned by a small set of basis functions. ROMs require a-priori data to complete the offline stage which itself is computationally expensive since obtaining the data requires many nonlinear full-field simulations.

In the case of the eigenstrain-based homogenization method (EHM) [2], the offline stage involves solving a series of linear elastic microscale equilibrium problems to compute localization and interaction tensors. This approach is advantageous as nonlinear simulations are avoided, but application to realistic microstructures still require further computational efficiency. In the first half of the presentation, we discuss application of the EHM to a polycrystalline microstructure with approximately 10,000 grains [1]. This microstructure was a part of the Challenge Problem 4 in the Air Force Research Laboratory's Additive Manufacturing Modeling Challenge Series dataset. Although EHM has been used to model elastoviscoplastic behavior of polycrystals with up to 1,000 grains using ROM sparsification strategy [2], further scaling of the method has previously been

limited by the cost of the offline stage. To overcome this limitation, an efficient model training strategy for EHM has been implemented. The proposed strategy utilizes a highly parallel implementation of an element-by-element conjugate gradient solver to evaluate the coefficient tensors. A key benefit of the proposed approach is that the assembly and storage of the stiffness matrix is not required in the evaluation of the influence functions. The conjugate gradient algorithm accelerated with parallel computing techniques results in rapid converges particularly when a suitable preconditioner is employed. Each discretized grain is treated as a separate domain and additional synchronization is used for nodes shared between several grains. The numerical experiments shows that while the CPFE simulation of the microstructure took about 44 hours using 640 processors on NASA's K-cluster, the online stage of the ROM took 20 minutes on a single core.

Although the online stage of the ROM is designed for efficiency, prior studies have identified inaccuracies in modeling both high-phase contrast and low-phase contrast materials. ROMs based on transformation field analysis typically deliver overly stiff response in comparison with direct numerical simulations. This effect is particularly pronounced in cases of high-phase contrast, such as composites subjected to transverse loading relative to the fiber orientation. To mitigate inaccuracies due to order reduction, a new affine EHM model is developed with the intention of using instantaneous moduli for recomputation of the instantaneous localization tensors [3]. The instantaneous moduli is incorporated in the formulation in order to better capture softening of the phases that enter plastic regime. The accuracy of the method is compared to the original EHM and direct crystal plasticity finite element simulations for several synthetic polycrystal microstructures, loading conditions and varying phase contrast. We show that the affine model delivers consistently softer response compared to the original EHM model. In particular, the affine model delivers notably more accurate response in the presence of high phase contrast. By enabling the recomputation of localization tensors, the affine EHM effectively captures local load redistribution, enhancing its predictive capability.

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A CONTINUUM-MICROMECHANICAL MODEL OF THE HUMAN STROMA

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Key words: Biological composite, Microstructure, human cornea, collagen network

Abstract. We present a numerical model of the human cornea where we combine a continuum model of the connective tissue of the stroma with a truss network that describes, at the mesoscale, the stiffening microstructure of collangen fibrils and chemical crosslinks.

The human cornea is a complex, highly specialized structure necessary for the vision function of the Eye. The cornea, due its shape and transparency, refracts and transmits the light to the retina. Cornea's mechanical properties, critical for maintaining corneal shape and function under intraocular pressure, arise from the composition of a hydrated proteoglycan-rich extracellular matrix (ECM) reinforced by an intricate network of collagen fibrils organized into lamellae. Despite extensive research, existing biomechanical models often fall short of capturing the coupled interplay between the ECM and collagen reinforcements, especially under physiological and pathological conditions. This work seeks to address this gap by proposing a novel computational model that integrates a continuum representation of the ECM with a discrete collagen-crosslinking network [1, 2, 3].

The continuum approach for the ECM is chosen to represent its viscoelastic behavior and interaction with fluid flow, critical for corneal hydration and load transmission. Conversely, the collagen network is modeled as a discrete, anisotropic reinforcement system, capturing the directional stiffness imparted by the collagen fibrils and their crosslinking. The model is developed in the view to account for the influence of enzymatic degradation,

age-related changes, and disease processes such as keratoconus, where alterations in the ECM-collagen coupling are known to drive structural instability.

The innovation of this approach lies in its multiscale integration, bridging the molecular mechanics of collagen crosslinking with macroscopic corneal behavior. By explicitly linking the continuum matrix with a collagen-reinforced network, the model offers some possibility to deepen our understanding of corneal mechanics. The inclusion of experimentally derived parameters for collagen alignment, crosslink density, and ECM properties, will make the model predictive in the simulation of physiological responses to intraocular pressure and external mechanical perturbations.

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MODELLING LIQUID UPTAKE, EXPANSION AND CURL OF PAPER SHEETS

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Key words: Porous media, liquid transport, swelling, dimensional stability

Abstract. In this study we aim to formulated models which, rooted in the micromechanics of the problem, allow one to predict the liquid uptake in paper sheets and the consequent out-of plane deformations of the sheets.

The dimensional stability of paper sheets may be severely affected by the ingression of water and other liquids. The underlying mechanism consists in the liquid entering the cellulose fibres and making them swell. The swelling fibres interact in the network, resulting in a certain degree of sheet-scale expansion. A gradient in the liquid content, and hence in the degree of swelling, through the thickness of the sheet results in curl, i.e. curvature of the sheet. Similarly, heterogeneity of the liquid content in the plane of the sheet may give rise to instabilities such as cockling and waviness.

The mechanics of these phenomena is understood reasonably well and predictive sheet scale models have been formulated – see e.g. [1]. These models generally assume the liquid content to be known as a function of space and time. However, many questions still surround the transport of the liquid (or in fact vapour) from the surface of the sheet into the fibres in its interior and truly predictive models are lacking. In this contribution we aim to address these challenges. We model the through-thickness liquid transport via the pore network by unsaturated flow, i.e. the Richards equation. A second balance equation governs the saturation of the fibres. The two equations are coupled by an exchange term. The constitutive relationships in the model, i.e. permeability, capillary pressure and exchange as a function of pore and fibre saturation are formulated based on micromechanical arguments together with a measured pore size distribution. The

fibre saturation is assumed to drive the expansion of the material and a simple elastic swelling model is adopted to predict the amount of curl as a function of time as the liquid penetrates the sheet and fibres. Predictions made by the model are compared with measurements made in immersion testing as well as curl testing.

In the second part of the presentation we assess the accuracy of assumptions made on the mechanics of the problem in sheet-scale continuum models [2]. An idealised, three-dimensional periodic fibre network model is taken as a reference. Effective mechanical and hygro-expansive properties of the network are determined under uniform wetting conditions. These effective properties are subsequently employed in a continuum model which is subjected to a through-thickness moisture gradient. The degree of curl predicted by the homogenised continuum model is compared against full-scale simulations of the discrete network model subjected to the same moisture gradient. The two approaches show a good agreement, confirming that the continuum approximation is valid even though the network has only 10 fibres across the thickness. If, however, the homogenised properties are determined using a two-dimensional version of the network model, a discrepancy arises due to the assumptions made in reducing the model to two dimensions.

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EFFICIENT MULTISCALE SIMULATIONS OF ADDITIVELY MANUFACTURED ALLOYS: TOWARD A HYBRID APPROACH COMBINING FE^2 AND FE-NN

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Key words: finite element squared, neural networks, multiscale simulations

Abstract. Poster contribution for *ECCOMAS CMCS 2025 Conference*.

Metafor [1], our in-house nonlinear finite element software, now efficiently performs finite element squared (FE^2) [2] simulations thanks to optimisations such as parallelised microscale FE analyses, macroscopic tangent moduli obtained from static condensation of the microscale using two (2D) or three (3D) nodes, and other numerical enhancements. Despite these improvements, the inherent computational cost of FE^2 remains a challenge.

Neural networks (NNs) have emerged as surrogates for microscale modelling, leading to the FE-NN paradigm as an alternative to FE^2. While faster, this approach requires substantial offline training and struggles with path-dependent material behaviours, where all possible loading paths must be considered. Addressing this often demands complex architectures (RNNs, GRUs, LSTMs), datasets, etc., further increasing training costs.

To overcome these limitations, we propose an original hybrid approach combining FE-NN and FE^2. A simple feedforward NN, trained on a well-defined dataset, efficiently handles known loading scenarios. When encountering an unseen path, the code dynamically switches from the NN to a finite element analysis for the microscale, i.e., from FE-NN to FE^2. This adaptive mechanism operates independently at each macro Gauss point, ensuring both accuracy and efficiency. At the end of the multiscale simulation, most of the macroscale domain has benefited from NN's speed, while only critical regions switched, at some point, to a classical FE analysis. This strategy optimises computational cost while providing detailed insights into microstructural behaviour in critical regions.

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SYMMETRY-ENFORCING NEURAL NETWORKS WITH APPLICATIONS TO CONSTITUTIVE MODELING

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Key words: Constitutive Modeling, Equivariance, Neural Networks

Abstract. The use of machine learning techniques to homogenize the effective behavior of arbitrary microstructures has been shown to be not only efficient but also accurate. In a recent work, we demonstrated how to combine state-of-the-art micromechanical modeling and advanced machine learning techniques to homogenize complex microstructures exhibiting non-linear and history dependent behaviors [1]. The resulting homogenized model, termed smart constitutive law (SCL), enables the adoption of microstructurally informed constitutive laws into finite element solvers at a fraction of the computational cost required by traditional concurrent multiscale approaches. In this work, the capabilities of SCLs are expanded via the introduction of a novel methodology that enforces material symmetries at the neuron level, applicable across various neural network architectures. This approach utilizes tensor-based features in neural networks, facilitating the concise and accurate representation of symmetry-preserving operations, and is general enough to be extend to problems beyond constitutive modeling. Details on the construction of these tensor-based neural networks and their application in learning constitutive laws are presented for both elastic and inelastic materials. The superiority of this approach over traditional neural networks is demonstrated in scenarios with limited data and strong symmetries, through comprehensive testing on various materials, including isotropic neo-Hookean materials and tensegrity lattice metamaterials. This work is concluded by discussing the universal approximation properties of the proposed architecture.

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AN EFFICIENT HOMOGENIZATION FRAMEWORK FOR SIMULATION OF NONLINEAR BENDING BEHAVIOR OF SPIRAL STRANDS

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Key words: Spiral strands, Non-linear hysteretic behavior, Computational homogenization

Abstract. Multilayer spiral strands are essential in applications like offshore wind turbine anchors and overhead power transmission. While individual wires behave elastically, the strands exhibit nonlinear hysteretic bending due to interlayer friction. Due to the large number of steel wires making up these strands, and to the nonlinear frictional contact interactions ruling the hysteretic behavior of such structures, direct numerical simulations (DNS) are extremely time-consuming in terms of computation.
This research develops an efficient framework to model spiral strands as equivalent beams, enabling accurate predictions of both global (moment-curvature) and local (axial stress variations within wires) responses. A mixed stress-strain-driven computational homogenization method is introduced to characterize the non-linear mechanical response at macro-scale by performing simulations at micro-scale on a short sample of strand considered as a representative volume element. This approach also enables virtual experiments to explore previously unexamined load scenarios with low computational cost.
Additionally, low-cost estimators for global and local responses are incorporated into the framework, allowing the equivalent beam model to be solved in seconds on standard laptops, compared to weeks required for performing DNS on supercomputers.
The proposed framework provides a practical and efficient solution for fatigue life analysis and complex loading scenarios in industrial applications.

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STRAIN LOCALIZATION ON EARTH: FROM MICROSTRUCTURAL HETEROGENEITY TO MACRO- AND MESOSCALE SHEAR ZONES

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Keywords: Strain localization, Geosciences, Anisotropic softening

Abstract. Strain localization is the rule rather than the exception in the deformation of the shallow layers of the Earth. Yet, modelling spontaneous strain localization in the viscous regime, which prevails on the lower 2/3 of the ~100km thick plates that form the outer shell of our planet, remains a real challenge. Observations and experimental work in shear zones, which are the expression of said strain localization, show that heterogeneity in composition and/or microstructure is key for strain localization. This heterogeneity exists at all scales, in particular small ones, and evolves in response to strain-rate and stress fields. In the ERC RhEoVOLUTION, we propose that poor representation of these heterogeneities and their evolution during deformation is the locking point for generating strain localization in geodynamical models. We examine how strain localization may arise in rocks deformed by viscous processes by associating a stochastic description of the mechanical properties of the medium with simple laws describing how these properties evolve in response to the resulting spatial variations in stress and strain-rate. These models show that initial heterogeneity in the rheological behavior and damage/healing due to evolution of the microstructure leading to spatial variations in the mechanical behavior controlled by the mechanical dissipation field are necessary, but not sufficient conditions to produce strain localization during viscous deformation. An additional condition is that the rate of energy consumption by the damage process is within a range from the average dissipation rate in the system. Based on these results we construct a regime diagram for viscous strain localization and parameterize the macro-scale response in the different regimes. Even if the microscale rheology is isotropic, strain localization due to dissipation-rate controlled microstructural damage results in emergence of anisotropic softening at the coarser scales. Ongoing work focus on the application of these results to model strain localization at the plates scale. *This work was supported by the European Research Council (ERC) under the European Union Horizon 2020 Research and Innovation programme [grant agreement No 882450 – ERC RhEoVOLUTION.*

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An advanced open-source toolbox for reducing computational costs: Civil Engineering Application

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Key words: OpenFOAM, Python, fvm, damage, cracks, concrete, plasticity

Abstract. This work provides a new open-source toolbox called SiCaR with high accuracy, robustness, and fast computation. The code is based on the language of OpenFOAM and new scripts written in Python. In the last decades and in the field of civil engineering, authors have focused on the development of constitutive model for concrete damage and cracks. Most authors have neglected the need to reduce computational cost and parallel time calculation. After damage, a new crack is generated at each time step and the topology of the initial mesh is changed, which increases the computational time. To reduce the computational cost, a new constitutive inelastic-plastic damage model has been developed based on the damage-plasticity model CDPM2 [1] and fracture mechanism [2, 3] implemented as a multiple hidden layers in the code SiCaR. To simulate crack propagation in damaged concrete structures, a new program written in Python has been developed to generate a mesh of crack patterns in their realistic state. This is an original work in civil engineering application and can be used for other problems such as crack propagation in metal after fatigue. Table 1 shows some important results of computational efforts, and figure 1 presents the use of Python scripts and OpenFOAM programming language to generate virtual 3D mesh of cracks starting from real 2D images. This numerical tool is used to simulate and validate predictions of remaining service life of damaged underground walls made with plain concrete. The predictions are compared with data obtained during the last 50 years ago.

Cases	Mesh size	CPU	SiCaR
Case 1	2k	1	6-8s
Case 2	80k	1	4-6min
Case 3	1M	20	15-20min

Table 1: Example of the computational costs

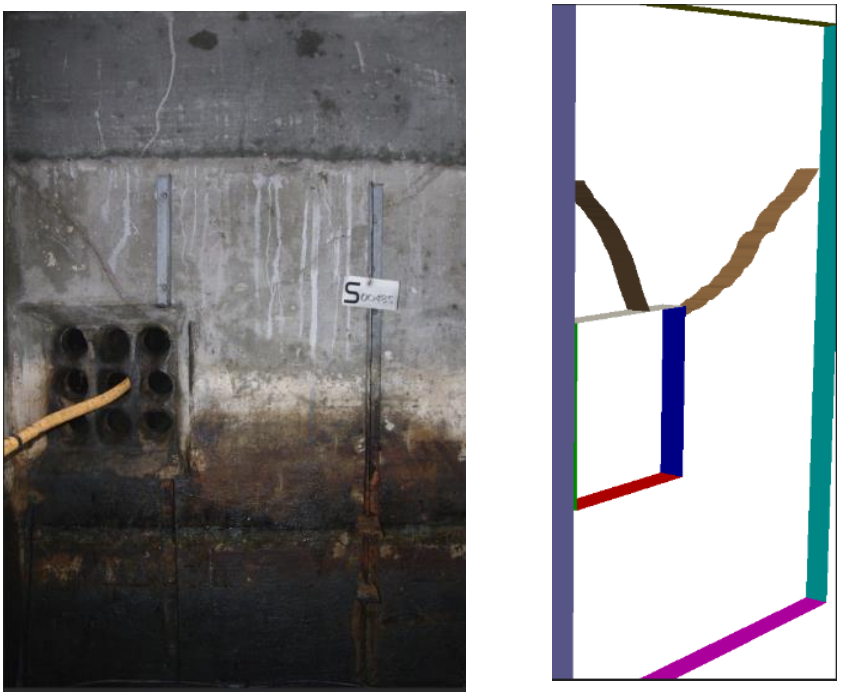

Figure 1: Crack patterns from reality (left) to virtual mode (right)

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Peridynamic modeling and mechanical characterization of material extrusion 3D-printed components

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Key words: Additive manufacturing, Peridynamic Theory, Process Parameters, Computational Modeling

Abstract

Additive Manufacturing Material Extrusion is widely used for producing complex and customizable structures through a layer-by-layer deposition process [1]. Besides all its benefits, predicting and optimizing the mechanical performance of these products remains a significant challenge due to inherent porosity, micro-cracks and inhomogeneity. Furthermore, inter-strand debonding due to weak connection between strands is a key factor in understanding the behavior of these parts. A model based on peridynamic theory is proposed to study the mechanical behavior of parts produced by 3D printing. By leveraging the advantages of Peridynamics [2,3], and its ability to define different interactions between material particles within strands and between strands, the heterogeneity of the material, particularly in the inter-strand region, is effectively considered. The results of the simulations were compared with data available in the literature and new tensile tests carried out in the laboratory [4,5]. Process parameters such as air gap, printing speed, extrusion speed, and layer thickness, were considered and the effect of these parameters on mechanical properties was evaluated. This integration of experimental activities and the development of numerical models provides a robust framework for predicting the properties of material extrusion AM components, paving the way for parameter optimization and material-specific design.

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GENERALIZED INTERFACES MODELING ADHESIVES AND THEIR FAILURE

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Key words: Anisotropic cohesive zone, Interface (in)elasticity, Generalized interface

Abstract.

The application of adhesive bonds in industrial production has been steadily increasing for decades. Finite-thickness adhesive layers can be approximated by zero-thickness interfaces for computational efficiency. Since adhesive layers show resistance and failure under tension, shear and in-plane stretch, a classical cohesive zone model is not sufficient to represent an adhesive. In contrast, generalized mechanical interfaces allow for displacement jumps under tension and shear loading, as well as, for traction jumps crucial for an in-plane response. Generalized interfaces at finite strains depend not only on the displacement jump and interface deformation gradient, but also on the spatial interface normal to account for anisotropic decohesion in a thermodynamically consistent model. In addition to a mode dependency in adhesives, experiments and micro-to-macro simulations in literature observed interactions between normal, shear and in-plane modes.

In order to take these effects into account, we present thermodynamically consistent, generalized interface models [1, 2] which allow for anisotropic decohesion, a membrane formulation and coupling of the damage modes. Numerical examples of brittle and soft adhesives demonstrate the performance and versatility of our models.

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DATA-DRIVEN MECHANICS OF SOFTENING MATERIALS

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Key words: Data-Driven Computational Mechanics, Lipschitz regularization

Abstract. In this contribution we discuss regularization strategies adapted to (model-free) data-driven approaches to softening material response. We look in particular to non-local/higher-order methods based on strain gradient or generalized continua

The data-driven computational mechanics (DDCM) paradigm of Kirchdoerfer and Ortiz [1] allows to perform numerical simulations directly from material data (strain-stress pairs), avoiding the need for an explicit constitutive model and identification of associated parameter. The method has been successfully applied to several non-linear and history-dependent classes of constitutive response [2].

It is well established that softening material response can lead to difficulties when solving boundary-value problems, such as loss of unicity and/or spurious mesh dependency in FE solutions. These difficulties remain in the DDCM context. These difficulties can be interpreted as stemming from the lack of a characteristic length, which has motivated the development of non-local/higher-order approaches to regularize the effects of softening. Most non-local approaches are based on gradients of the internal variable associated to softening (damage, plastic strain, ...), but DDCM typically avoids to introduce such internal variables. It is thus necessary to apply regularization on the observable state variables such as strain and/or stress.

We will thus discuss different approaches to introduce non-local/higher-order regularization within the DDCM framework, such as Lipschitz regularization [3] or generalized (micromorphic) continua [4], and illustrate them on representative examples.

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CANONICAL INTERFACES WITH APPLICATION TO MICRO-HETEROGENEOUS SOLIDS

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Key words: Interface modeling, Computational homogenization

Abstract. This contribution concerns some recent developments of interface modeling and its role in computational homogenization, [1]. Focus is primarily placed on purely mechanics problems.

Finite-thickness interphases between different constituents in heterogeneous materials are often replaced by a zero-thickness interface model. Typical examples are the transition zone between inclusion and matrix in composites or the grain boundaries in polycrystalline solids. Due to increasing area-to-volume ratio with decreasing size of microstructures, interfaces introduce a physical length into the effective response at the macroscale. In terms of purely mechanical response, the most commonly studied interface models are the *cohesive interface model* and the *elastic interface model*. In a series of papers, Javili and coworkers, e.g. [2], discussed various options to generalize these (extreme) model versions.

In this presentation, we discuss a novel *canonical interface model* based on a variationally consistent approach, which encompasses all previous interface models for the purely mechanical problem, [1]. Moreover, variationally consistent homogenization is employed to upscale an elastic composite with particle/matrix interfaces. The numerical results highlight the significance of the canonical interface model on the overall response of composites, at times leading to counter-intuitive behavior at the macroscale.

In the basic approach, the constitutive properties assigned to the interface are phenomenological. However, it is possible to account for the micro-structural features in a thin interphase zone and employ geometrical reduction and homogenization to *derive* the interface properties. In particular, it is possible to account for "unconventional" micro-design within the interphase to bring about meta-material characteristics upon upscaling.

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RBF-BASED SURROGATE COMPUTATIONAL HOMOGENIZATION FOR 3D INELASTIC COMPOSITES

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Key words: Computational homogenization, Surrogate model, RBF interpolation, Localization

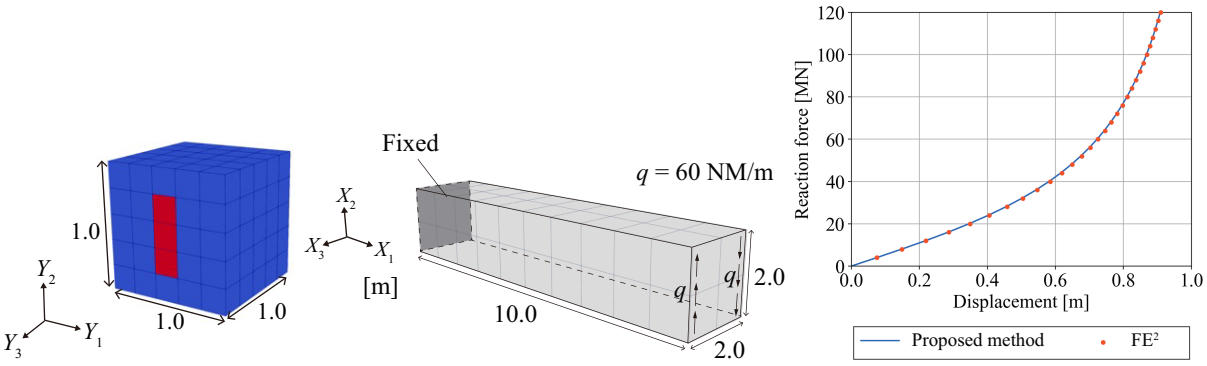
Abstract. Three-dimensional surrogate computational homogenization using radial basis function interpolation are pursued for composite materials that exhibit inelastic behavior, such as elastoplastic and viscoelastic.

Data-driven methods for computational homogenization (CH) have been studied to overcome the difficulty of conventional multiscale analysis methods. In particular, a variety of data-driven approaches have been developed for history-dependent materials such as elastoplastic composites [2], but to the best of our knowledge, most of the studies are based on neural networks (NNs). Although there is no doubt about the power of NNs, the input-output relationship is a black box, not allowing for our understanding of mechanical correspondence. To avoid such an invisible process, we have recently proposed a class of surrogate CH using radial basis function (RBF) interpolation [1], which substitutes for the microscopic analysis for inelastic composites at small-strain and finite-strain [3, 4]. However, the computational cost of the process of obtaining the weights of RBFs by solving linear equations with the kernel matrix as coefficients is high, and this approach has been applied only to two-dimensional (2D) problems.

To address the above issue, in this study, various measures will be taken to extend the RBF-based surrogate CH to 3D problems from a practical perspective. In the first simple measure, a limited number of combinations of the six components of macroscopic strain are randomly selected on the hypersphere to perform numerical material tests to generate a set of macroscopic stresses and macroscopic strain histories. After that, the procedure should be the same as the one we have developed so far.

As an example of numerical analysis, let us apply it to a composite material consisting of hyperelastic materials. Fig. 1 (a) shows the unit cell, where the Neo-Hookean constitutive law is employed for both the matrix and the inclusion. The Young's moduli of matrix and inclusion

are set to $E = 1.0 \times 10^3, 1.0 \times 10^5$ MPa, respectively, and the Poisson ratios are commonly set to $\nu = 0.2, 0.3$. Taking the measure described above, we created a surrogate CM model and conduct a macroscopic analysis for the structure shown in Fig. 1 (b). Fig. 1(c) shows the load-displacement curves obtained on the loaded surface compared to the FE^2 result. This graph shows the result of proposed method is good agreement with that of FE^2.



(a) Unit cell (b) Macroscopic finite element model (c) Load displacement curves

Figure 1: Unit cell and macroscopic problem

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PHYSICALLY RECURRENT NEURAL NETWORKS APPLIED TO MULTISCALE ANALYSIS OF THERMOPLASTIC COMPOSITES

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Key words: Physics-informed machine learning, multiscale analysis, composite materials

Abstract. The response of fiber reinforced composite materials can be described accurately on the microscale, combining constitutive models that capture the physics of the constituents with a geometric representation of the microstructure, such that orthotropic behavior emerges. For composites with a thermoplastic matrix, the relevant physics includes visco-elasticity and visco-plasticity, which is challenging to represent directly in an orthotropic constitutive model, while detailed descriptions do exist for the pure polymer, such as in the Eindhoven Glassy Polymer (EGP) model [1].

In recent work, we have used the EGP as constitutive model for the matrix in a micromodel aimed at describing rate-dependent failure [2] and creep and fatigue of thermoplastic composites [3]. To explore the ability of the micromodel to describe the response of the composite material for different stress states, off-axis tests were analyzed. The micromodel could accurately reproduce various trends in the experiments, but for experiments with small off-axis angles the model failed to reproduce even the pre-peak nonlinear response. It was hypothesized that the observed mismatch could be due to macroscopic variations in the experiment. Because boundary conditions in the experiment do not allow for shearing of the specimen, the macroscopic stress state is not uniform for specimens with fiber orientations other than 0°and 90°. Consequently, information is lost when the experiment is modeled with a single micromodel.

In this presentation, the experiments are analyzed in a multiscale framework, focusing on the pre-peak response. Because computation times for a fully coupled multiscale analysis would be prohibitively high, a data-driven surrogate is used to accelerate the analysis. Specifically, we use the Physically Recurrent Neural Network (PRNN). The core idea of the PRNN is that the constitutive models from the original micromodel are embedded in the hidden layer of a neural network (see Fig. 1). The resulting surrogate generalizes very well with limited training data, with as most notable example that it can reproduce unloading and reloading behavior without having seen it during training [4].

We use a rate-dependent large-displacement version of the PRNN that includes the EGP in the hidden layer to perform simulations of the off-axis experiments from [2]. The off-axis test is modeled on the macroscale, where stresses are computed from the PRNN that is trained on data from a micromodel. It is shown that for small off-axis angle, the multiscale simulations are more accurate in reproducing experimental measurements than the pure micromodel simulations, without compromising accuracy for large off-axis angles, confirming the hypothesis that macroscopic variations are significant in the experiment for small off-axis angles.

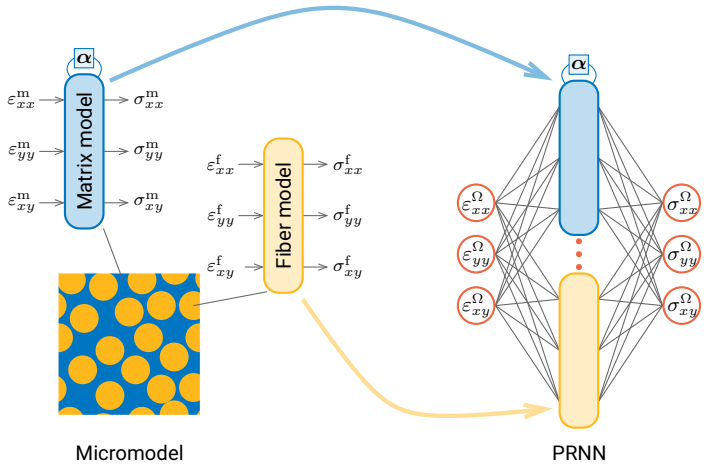

Figure 1: Physically Recurrent Neural Network with constitutive models in the hidden layer of a neural network.

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MULTISCALE MODELING OF HEAT TRANSFER IN GRAPHENE-COPPER NANOCOMPOSITES

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Key words: Heat conduction, molecular dynamics, additive manufacturing, graphene

Abstract. This study investigates the thermal properties of graphene-copper metal-matrix composites, resolving nanoscale structures through Non-Equilibrium Molecular Dynamics (NEMD) simulations and developing a continuum-upscaled model using homogenization. The continuum model is based on the NEMD findings and aims to predict the thermal properties of graphene-copper powders, which serve as feedstock material for Additive Manufacturing (AM).

Recent advances in AM have created new opportunities for realizing composite materials and novel parts with unique structures and properties. Here, the combination of graphene, a highly conductive two-dimensional material with an in-plane conductivity in the range of $[3000 - 5000]$ W/mK, with copper is studied for its mechanical and heat transfer properties. Images documenting the morphology of the graphene-copper composite powder are shown in Figure 1. However, accurately predicting the thermal and mechanical characteristics of the resulting material is challenging as the nanoscale interactions between the constituent elements on atomistic scales need to be translated to macroscopic material properties.

We have performed NEMD using LAMMPS [1, 2] to simulate the anisotropic thermal conductivity and interface resistance of graphene-copper nano-structures. Since research has shown that the thermal properties of interfaces are structure- and size-dependent [3], we have performed these simulations for various configurations. These are reference Representative Elementary Volumes (RVEs), Cf. Figure 2, on which upscaling should be

based. We aim to establish a reliable mesoscale model through homogenization based on nanoscale heat transport properties extracted from the RVEs of graphene-copper structures. Our poster will present findings from the heat transfer model, informed by nanoscale data, and features of the 3D reconstruction of the manufactured graphene-copper material.

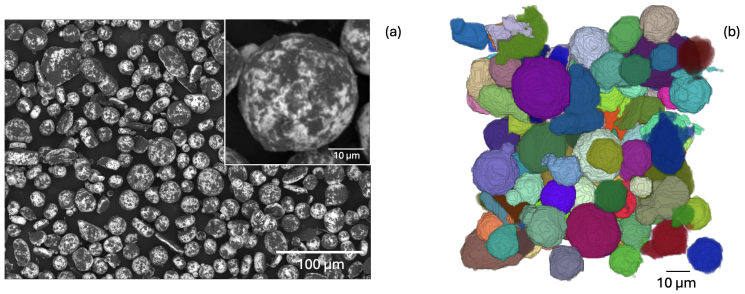

Figure 1: SEM image of Graphene-Copper powder (a) and 3D reconstruction of XCT data (b).

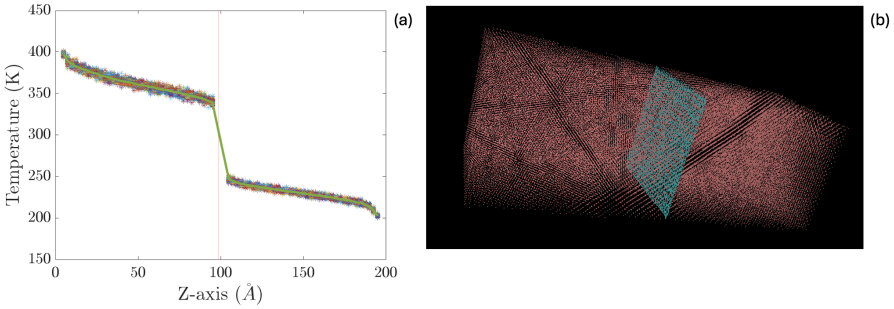

Figure 2: Temperature distribution (a) in NEMD simulations (b) of Copper-Graphene-Copper interfaces.

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MODEL ORDER REDUCTION FOR PARAMETRIZED TWO-SCALE SIMULATIONS

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Key words: model order reduction, computational homogenization, hyperreduction

Abstract. In order to optimally design materials, it is crucial to understand the structure–property relations in the material by analyzing the effect of microstructure parameters on the macroscopic properties. Unfortunately, the high computational costs of such multiscale simulations in computational homogenization often render the solution of design, optimization, or inverse problems infeasible. To address this issue, we explored and developed parametric model order reduction techniques to construct inexpensive surrogates for parametrized microscale problems. The method is specifically well-suited for multiscale simulations since the coupled simulation is decoupled into two independent problems: (1) solving the microscopic problem for different (loading, material, or geometric) parameters and learning a surrogate model from the data; and (2) solving the macroscopic problem with the learned model.

In this talk, we summarize several works on developing reduced order models for parametrized microstructures in the *data-poor* regime, i.e., for applications in which the amount of data (either through measurements or simulations) to be used for training must be economized. In the first part, we discuss a non-intrusive reduced basis method

[1]T. Guo worked on the project while he was affiliated with the Department of Mathematics and Computer Science at Eindhoven University of Technology.

to construct approximations for the microscopic stress field [1, 2]. The method is based on combining proper orthogonal decomposition (POD) and regression [1]; in the case of geometric parameters [2], an auxiliary problem is also used to treat the geometric transformations. The method permits accurate and efficient prediction of the microscopic stress field for a wide range of parameters, and can be readily used in design and optimization tasks. Numerical results show that the method achieves high accuracy and efficiency.

In the second part, we discuss intrusive reduced basis methods that permit the treatment of more complex behaviors. We present a method based on POD and the empirical cubature method [5] capable of treating nonlinear history-dependent behaviors. Numerical tests illustrate the significant speed-ups and accuracies achieved while observing good extrapolation behavior. Finally, we present a technique [4] that combines reduced basis methods with second-order computational homogenization, thus allowing to capture nonlinear behaviors arising from nonlocal interactions (e.g., due to buckling or patterning of the microstructure). Numerical examples compare the reduced solutions with respect to direct numerical simulations and the full second order computatational homogenization model. Results show the potential and efficiency of the proposed method.

Acknowledgment. This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 818473).

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SCALE TRANSITION BEHAVIOR OF PHASE TRANSFORMING SOLIDS

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Key words: Variable Scale Separations, Homogenization, Phase-Field Modeling

Abstract. The homogenization of materials with a fixed microstructure has been a major focus of research over the past decades. However, homogenizing phase-transforming solids, which exhibit evolving microstructures, still remains an unresolved problem, even at the methodological level. In fact, the conventional definition of scale separation based on the wavelength of fluctuations in material properties cannot be applied in this context. This is because these fluctuation's lengths change over time when considering phase transforming solids. An appropriate characterization of representative volume elements is thus almost impossible if the microstructure evolves heterogeneously.

To overcome these issues, the new concepts of phase-morphology and variable scale separations were recently introduced in [1, 2] as a fundamental homogenization framework for phase transforming materials. More specifically, in contrast to conventional homogenization theories, the ratio between micro- and macroscopic scales is now defined through a scale separation factor, which is independent of any wavelength of property fluctuations, and can therefore be chosen arbitrarily. This allows, for instance, the analysis of effective system driving forces, the evolution of martensite laminate reorientation as well as the coupling between variable spatial and temporal scale separations — all based on a collection of nonlinearly weighted phase averages. The validity of the presented results is verified by two-dimensional finite element simulations of martensite formation in a ZrO_2-like dual-phase material. It is thus shown, that the outlined methodology provides and improved understanding of the scale transition behavior of phase transforming systems, even during the microstructure evolution process.

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AN EXTENDED ANALYTICAL MODEL FOR THE STATISTICAL STRENGTH OF QUASIBRITTLE MEDIA BASED ON EXCURSION STATISTICS OF RANDOM FIELDS

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Key words: Quasibrittle material random strength upscaling, Extremes, Averaging

Abstract. One of the fundamental behaviors of structural materials—particularly heterogeneous, quasibrittle materials such as concrete, ceramics, and various geomaterials—is the dependence of their mechani-cal properties on structural size. In this work, we build upon our recently developed analytical model [1] for the fracture behavior of concrete, which explicitly captures the size dependence of structural strength. This extension allows us to analyze not only uniformly stressed structures but also more general stress configurations arising from a variety of loading conditions. The model accounts for stress redistribution within the fracture process zone by averaging local stresses, and it compares this resulting effective strength to the averaged random field representing material strength. Analytically, we determine the probability that the nonuniform effective stress field exceeds the averaged strength field, thereby obtaining a comprehensive probability density function for the structural strength. This function naturally includes both energetic and statistical contributions to the overall size effect in quasibrittle materials.

We consider the local material strength to be a random property over the specimen volume, $f_t(\boldsymbol{x}) = H(\boldsymbol{x}) f_{t,0}$, where $f_{t,0}$ stands for the mean strength and $H(\boldsymbol{x})$ is a unit-mean random field varying over the specimen volume. We assume that the structural strength is exhausted when the load of a certain critical volume (called RVE) achieves its strength. This zone can appear at any location and its dimensions, related to fracture process zone, are assumed as known. Its strength is roughly taken as the average strength over its volume. Thus, we can as well consider strength of any potential critical volume inside the structure as the local average inside a sliding RVE volume

$$H_{\text{eff}}(\boldsymbol{x}, \text{RVE}) = \frac{1}{V_{\text{RVE}}} \int_{x \in \text{RVE}} H(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \tag{1}$$

which is also a random field, but with a reduced variance and modified autocorrelation structure, both obtainable analytically. By considering the effective stress field $\sigma_{\text{eff}}(\boldsymbol{x})$, e.g., as an average stress in the above-mentioned critical volume, we can formulate the probability that the structure fails for the given stress field $\sigma(\boldsymbol{x})$ as

$$G_{\text{f}}(\sigma(\boldsymbol{x})) = \text{P}\left(H_{\text{eff}}(\boldsymbol{x})_{\boldsymbol{x}\in\Omega} < \frac{\sigma_{\text{eff}}(\boldsymbol{x}) - \mu_{\text{eff}}}{\delta_{\text{eff}}} \right) \tag{2}$$

which is the cumulative distribution function of strength of the considered concrete structure or specimen occupying region Ω. Its statistical moments can be easily derived from the distribution function $G_{\text{f}}(\sigma(\boldsymbol{x}))$. In our previous work [1], we were able to provide analytical solution to the distribution function of strength for approximately constant stress field, and application of the model to situation with stress concentration must have been preceded by analysis of effective size of domain with a constant strain. In this contribution, we present a generalization to nonuniform stress fields $\sigma_{\text{eff}}(\boldsymbol{x})$. The evaluation of the probability distribution involves a simple integral that must be computed numerically, but the computation is very effective.

This extension increased the applicability of the model to much wider stress configurations. The model captures the energetic/statistical size effect behavior and it asymptotically tends to the classical Weibull-type dependence of strength on structural size, which disregards strength redistribution and spatial correlation of local strengths. Increase in the RVE volume reduces the variance of structural strength and decrease also the rate of average strength with size. Its validation will be performed by using an experimental series with a broad size range—a famous experimental series conducted on dog-bone specimens [2, 3, 4].

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RECENT DEVELOPMENTS ON PHYSICS-AUGMENTED NEURAL NETWORKS FOR MATERIAL MODELING

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Key words: Neural networks, hyperelasticity, thermo-elasticity, dissipation, damage, polymers, optimisation, nonlinear beams

Abstract. In recent years, various data-driven and machine learning approaches have been proposed for the modelling of microstructured materials subject to large deformations, dissipatitve, and multi-physical material behaviours. However, as commonly observed in machine learning, purely data-driven methods and in particular neural networks suffer from poor generalisation and extrapolation, and require large amounts of data for training. As a remedy, *physics-augmented* machine learning aims to incorporate prior knowledge into the formulation of data-driven models, thus ensuring physically sensible and robust predictions.

In particular for constitutive modelling, we have proposed *physics-augmented* neural networks (PANNs) that ensure all theoretical requirements of hyperelasticity [1, 2]. We have demonstrated their ability to be trained on scare data, their applicability to microstructured materials, their robust performance in finite element simulations, as well as their extensibility to electro-elasticity [3].

In this presentation, we would like to introduce further recent developments around PANNs, including:

- Parameter-dependent PANNs for hyperelastic material behaviours [4].
- Application of such parameterised models for nonlinear multiscale topology optimisation of microstructured materials.
- Hyperelastic PANNs with relaxed convexity criteria based on monotonous NNs, which offer more flexibility to fit highly nonlinear material behaviours but nevertheless perform very robustly [5].
- PANNs for thermo-elasticity with convex-concave functional requirements [6].

- Generalised standard materials and other theoretically guided PANN architectures for inelastic, dissipative material behaviours, including visco-elasticity and hyperelasticity with damage (Mullins effect).
- PANN formulations for nonlinear material behaviours in structural mechanics, in particular for geometrically exact beams [7].

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A CLUSTERING APPROACH TO ACCELERATE FE^2 ANISOTROPIC FRACTURE SIMULATIONS

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Key words: Fracture, Multiscale, Clustering

Abstract. An approach is proposed [1, 2] to accelerate multiscale simulations of heterogeneous quasi-brittle materials exhibiting an anisotropic damage response. The present technique uses unsupervised machine learning classification based on k-means clustering to select integration points in the macro mesh within an FE^2 strategy to remove self-similar micro nonlinear problems and to avoid unnecessary Representative Volume Element (RVE) calculations.

More specifically, a classification vector including strains and internal damage variables is defined for each macro integration point. The macro internal damage variables are constructed using harmonic analysis of damage. At each step of the macro iterations, the integrations points are grouped into clusters and only one nonlinear problem is solved for each cluster. As a result, the computations are accelerated within an FE^2 scheme by reducing the total number of RVE problems to be solved. The developed algorithm includes a macro regularization and an arc-length technique to capture macro snap-back due to the softening. Applications are proposed to simulate the response of different heterogeneous quasi-brittle materials with strong anisotropic responses. speed-up factors of the order of 12 to 15 can be achieved without the need to build a database, and without reduced-order modelling approximations at the micro level. Estimates of structural strength can be obtained with Speed-up factors between 45 and 85.

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PREDICTING TEXTURE-INDUCED ANISOTROPY IN THE EARTH'S MANTLE USING SUPERVISED DEEP-LEARNING

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Keywords: anisotropy, texture, geophysics

Abstract. Olivine, the orthorhombic mineral composing 60-80% of the upper mantle (the layer between 10-30km and 410 km in the Earth), has a strong intrinsic elastic and viscoplastic anisotropy. It also develops strong textures in response to viscoplastic deformation, which results in elastic and viscoplastic anisotropy at much larger scales, of up to 100s of km. Predicting the evolution with strain of texture-induced mechanical anisotropy in the mantle is essential to: (1) probe indirectly the deformation (due to thermal convection) in the mantle with seismic measurements and (2) account for memory in simulating the long-term deformation of the Earth. However, traditional micro-mechanical approaches to model the evolution of this texture-induced anisotropies are too memory-costly and time-consuming for coupling into geodynamical simulations. To speed up the prediction of elastic anisotropy in the mantle, we develop deep-learning (DL) surrogates trained on a synthetic database built with viscoplastic self-consistent simulations of texture evolution of olivine polycrystals in typical 2D geodynamical flows. A first challenge was the choice of memory-saving representations of the texture. Training the DL models on the evolution of the elastic tensor components avoids the need of saving the texture itself. We tried different architectures, obtaining the best efficiency/accuracy ratio for multilayer feed-forward (FFNN). The results highlight the importance of (1) the standardization of the outputs in the training stage to avoid overfitting in predictions, (2) the statistical characteristics of the strain histories in the training database, and (3) the influence of non-monotonic strain histories on error propagation. Predictions for complex unseen strain histories are accurate, much more time-efficient and less memory-costly than traditional micro-mechanical models. Yet preventing error compounding in a recursive-prediction scheme – where the model prediction at a given time step becomes the input for the next step - to evaluate the anisotropy evolution along a flow line for long and complex deformation histories remains a challenge.

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FFT SOLVERS FOR COMPUTATIONAL MICROMECHANICS: ENHANCING NUMERICAL EFFICIENCY THROUGH PDE PRECONDITIONING PERSPECTIVE

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Key words: homogenization, FFT-based solvers, preconditioning, Krylov solvers

Abstract. Moulinec and Suquet's FFT-accelerated solvers are used widely in image-based computational micromechanics. This talk presents their reformulation as a finite element method with Laplace preconditioning, preserving the efficiency of the original formulation while removing Fourier ringing discretization artifacts.

The use of spectral trigonometric solvers in image-based computational micromechanics, first introduced by Moulinec and Suquet [1], has become widespread due to their computational efficiency, low memory requirements, and ease of implementation. In this talk, we will focus on the finite element (FE)-based reformulation of the original scheme, as pioneered by Schneider et al. [2] and Leuschner and Fritzen [3]. In particular, we will (1) provide a linear algebra perspective on their developments and (2) relate them to recent advances in Laplace preconditioning of elliptic partial differential equations [4].

The approach adopted [5] involves preconditioning the periodic cell problem using a discrete Green's operator derived from a reference problem with constant coefficients. Theoretical analysis shows that the eigenvalues of the preconditioned matrix can be bounded

from above and below by coefficients of the original and reference problems. This allows the system to be solved by the preconditioned conjugate gradient method in a number of iterations that is almost independent of the grid size. In terms of implementation, we take advantage of the fact that for generic arbitrary regular meshes, the system matrix of the reference problem has a block-diagonal structure in Fourier space and can be efficiently inverted using Fast Fourier Transform (FFT) techniques. As a result, the computational complexity of the scheme is dominated by the FFT, making it equivalent to that of spectral solvers. Unlike trigonometric spectral solvers, the proposed scheme works with arbitrary FE shape functions with local support and does not exhibit the Fourier ringing phenomenon.

If time allows, we will end the talk by exploring the potential of the proposed framework for integrating Greens' preconditioners with other preconditioners and for addressing non-uniform discretization grids.

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