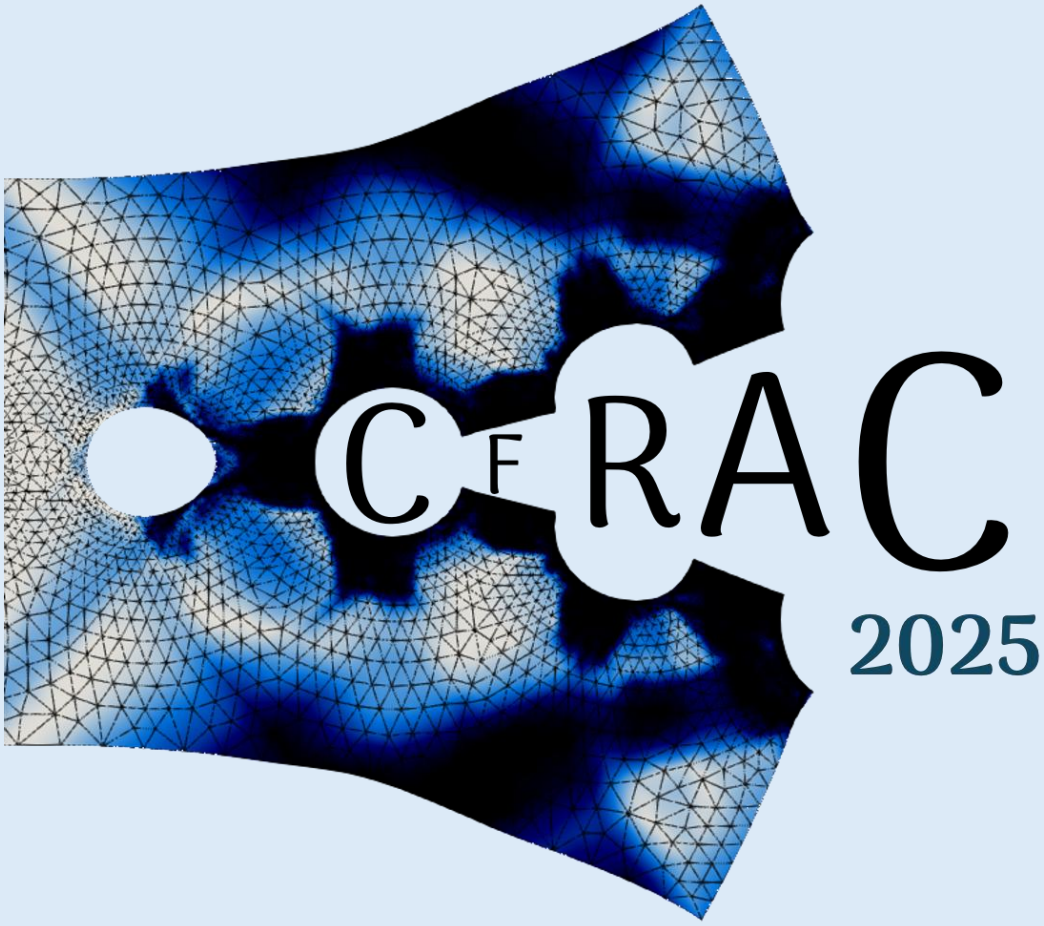

The Eighth International Conference on Computational Modeling of Fracture and Failure of Materials and Structures

Porto, Portugal, 4-6 June 2025

Edited by:
P.P. Camanho, N. Moës, L. De Lorenzis, M. Jirásek

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Porto, Portugal, 4–6 June 2025

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Preface

Following a series of successful editions in Nantes, Barcelona, Prague, Paris, and Braunschweig, the 2025 International Conference on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC) took place in Porto, Portugal, from June 4th to 6th, 2025. CFRAC is a thematic conference held with the support of the European Community on Computational Methods in Applied Sciences (ECCOMAS).

The primary objective of the CFRAC conference series is to bring together researchers and industrial partners engaged in the development and application of advanced numerical methods for simulating fracture and failure in materials and structures. The event aims to foster dialogue, facilitate the exchange of ideas, and promote collaboration among research groups across Europe and around the world with a shared interest in computational fracture mechanics.

This scientific domain plays a vital role in meeting the increasing demands for structural safety, reducing non-recurring costs in product development, and lowering the recurring operational expenses of complex engineering systems. As new materials and applications emerge, conventional design rules and experimental testing methods often fall short, highlighting the growing importance of computational methods in modern design and certification processes. The synergy between computational modeling and advanced experimental techniques is essential for accelerating innovation and optimizing product development.

CFRAC 2025 featured 15 mini-symposia focused on both traditional and emerging research areas, alongside five plenary lectures delivered by leading scientists in the field. The conference hosted a total of 172 presentations, delivered across eight parallel sessions. The proceedings include abstracts from all contributors and are organized into chapters corresponding to each mini-symposium.

The co-chairs gratefully acknowledge the invaluable contributions of the mini-symposia organizers, whose dedication continues to be instrumental in the success of the CFRAC conferences. Special thanks are extended to Prof. Albertino Arteiro (University of Porto) for his key role in organizing CFRAC 2025. We also appreciate the support of Dr. Francisca Alves and Dr. Nathan Klavzer (INEGI), along with PhD students Norá Kovács and Erdem Dinler (University of Porto), in preparing the proceedings. The support of EikoSim is also sincerely acknowledged.

The full proceedings are freely available for download on https://cfrac2025.pt/.

We hope readers will find this collection insightful and valuable for their research and professional endeavors.

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- V. Lazarus
- L. H. Poh
- J.-J. Marigo
- O. Allix

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Plenary Lectures

Ductile versus brittle fracture in refractory High Entropy Alloys: What can the atoms tell us?

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ABSTRACT

The brittle-ductile transition in refractory body-centered-cubic (bcc) metals and alloys has been an unresolved theoretical topic for many years. With the emergence of multi-component near-random bcc "high entropy alloys (HEAs)" that exhibit impressive high-temperature strength, the Achilles heel of brittle fracture at room temperature is among the most pressing issues to understand and resolve. Microscopy of fracture in the bcc elements Nb, Mo, and W suggests that dislocation emission from the crack tip is a critical phenomenon that enables crack blunting and prevents cleavage failure. The BDT is thus proposed to be associated an intrinsic brittle(cleavage)-ductile(emission) process at a sharp crack, which is then intrinsically atomistic. Here, the intrinsic brittle/ductile response is analyzed within linear elastic fracture mechanics to identify the relevant material properties and fracture orientations in bcc systems. Material properties are then computed using first-principles or atomistic potentials and a criterion for ductility is derived [1]. That criterion is then used to assess a wide range of HEAs with some success. Alternative criteria and concepts are also discussed and compared. The role of alloy disorder is analyzed and found to promote ductility, but a surprising reason. Incorporating the ductility criterion into an alloy-design process [3] identifies a promising family of Hf-Mo-Nb-Ti HEAs with high strength, high temperature strength, and possibly sufficient ductility. Nonetheless, we also report on HEAs that show a typical ductile failure mode but have very modest tensile ductility, highlighting the need to go beyond BDT criteria in the development of suitable high-performance bcc HEAs.

Perturbative approaches to study the propagation of complex-shaped cracks

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ABSTRACT

One way to contribute to the urge of climate transition in the field of fracture mechanics, is to affine predictions of damage tolerance approaches used to assess the durability and fiability of sensitive components (aero-nautics and -space, nuclear industry): if it can be certified that reduced safety are safe, the interval between maintenance operations could be increased and the replacement of defective parts be delayed, hence their environmental footprint be reduced. The aim of Damage Tolerance Approaches is to ensure that the existence of unavoidable defects will not compromise the safety of people. It consists in placing oneself in the most unfavorable case of brittle fracture and to determine the propagation of a preexisting crack under cyclic loading until the Griffith brittle fracture threshold is reached. At present, it is done using simplified smoothed out crack geometries, either using tabulated values or Finite Element Methods. As the meshing of the entire structure is required, the latter are currently unable to accurately account for small scale tortuosity of crack geometry. During this presentation, I will show that perturbations approaches are efficient alternatives to address this challenge. In addition to the seek of refined safety margins, they also permit to ensure that small geometrical perturbations will not lead to unexpected catastrophic failure. Perturbation approaches aim to provide analytical formulas for the variation of the stress intensity factors arising from small scale perturbations of the crack shape, simplifying the macroscopic aspects of the component. I will focus on two applications in which taking into account small scale features of the crack geometry leads to increased apparent toughness. In the first, it results form arbitrary crack front distorsion from circularity in the second by the formation of facets in mode I+III brittle fracture.

The localizing gradient damage model for dynamic fracture

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ABSTRACT

The conventional gradient enhancement has been widely used to resolve mesh sensitivity issues during strain softening. However, it may induce a spurious damage growth phenomenon. This motivates the development of the so-called localizing gradient enhancement where the nonlocal interaction decreases with damage in the free energy statement. The ensuing balance equation resembles that of the conventional gradient enhancement, albeit with a higher order flux term that vanishes with damage. The localizing gradient enhancement has been adopted for different damage and/or plasticity models in quasi-static conditions and has been shown to give localized damage profiles at failure. In this presentation, we focus on the use of the localizing gradient damage model for dynamic fracture. Particularly, we consider the incorporation of a micro-inertia term in the nonlocal balance equation and discuss on the influence of this additional term on the model predictions. To facilitate an ease of use of the model, a simple numerical implementation in the commercial software ABAQUS will also be presented, by adopting the built-in thermal-mechanical elements, and the results benchmarked against available experimental data in the literature.

On the modelling of the crack nucleation by the variational approach to fracture

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ABSTRACT

It is well known that the nucleation of cracks is not possible with Griffith's theory of fracture essentially because in that theory the stresses are not bounded. Gradient damage models or more generally phase field models have been introduced to compensate for this lack. Their construction follows a variational approach which is based on clear physical principles, allows rigorous mathematical results and facilitates its numerical implementation. However, the most used models of this type like Ambrosio-Tortorelli' model leads to too simple strength criteria. Moreover the size of the yield stress surface depends on a parameter which tends to infinity when this parameter goes to zero. Therefore, those phase field models must be improved. In the talk, we will see as it is possible to construct phase field models such that the yield stress surface be as general as possible (with the unique restriction to be convex) and the size of which remains finite when the small regularizing parameter tends to zero. For that, it is not necessary to leave the comfortable variational approach and we will even show that the variational approach makes it possible to obtain a limit model which is entirely coherent. In particular the procedure will be developed for the construction of a model of fracture of an initially incompressible material which contains a fix limit for the spherical part of the stress tensor.

Extension of quasi-static damage meso-modelling of composite laminates to dynamic failure and erosion

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ABSTRACT

Impact tests on structures are destructive, costly and difficult to analyze. This is particularly true for composite structures, whose properties and failure mechanisms are highly dependent on the chosen stacking architecture. As a result, virtual testing is of paramount importance for the design of composite structures subjected to impact ... but difficult.

Because of the practical importance of laminated composites, and thanks to fifty or more years of intensive research, the response to static failure is now well understood. At the meso level, this involves microcracking, fiber breakage, delamination and their interaction. Since the damage mechanisms typical of laminated composites with continuous long fibers are the same in both static and dynamic conditions, we can hope to extend the static meso-modeling of laminated composites to the dynamic.

Another aspect is that, in today's industrial environment, due to the lack of robustness of the local constitutive model, important numerical parameters such as mesh density are fixed in order to calibrate the model against a reference test. This process is tedious, and only allows the safe analysis of variations around well-controlled situations. The most widespread approach to overcoming the lack of consistency of the material model with regard to fracture is that of non-local spatial approaches, including phase-field approaches. In the case of composites, where numerous scales and mechanisms need to be addressed, these methods have yet to be developed and validated.

We therefore tried another possibility, that of regularization using a time-dependent model, which is quite natural in dynamics. It appears that using a usual rate-dependent model is not sufficient to circumvent all the problems associated with spurious damage localization in the dynamics. This is why we have proposed and developed the concept bounded rate damage model. A consequence of the model is that a minimum critical time is required to completely damage the material. The coupling between time and space seems to prevent parasitic localization, at least in our experience to date.

The presentation will cover these aspects, the basis for meso-modeling laminate damage and the limited damage rate model, as well as some applications and adaptations to dynamic delamination and damage, fracture and erosion of laminates subjected to high-speed impact.

Minisymposium DDF:

Data, damage and fracture

Organized by P. Carrara, C. Jailin and I. Rocha

A phase-field anisotropic model for the multiscale analysis of short fiber reinforced polymers

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ABSTRACT

Understanding and modeling the fracture mechanical behavior of short glass fiber reinforced polymers (SFRPs) is challenging: the strong heterogeneity induced by the manufacturing process causes a tight coupling of the material microstructure to the effective response on the component scale. Aiming to account for this microstructural complexity, fracture is approached using a multiscale approach.

Typically manufactured via injection moulding, SFRP components exhibit locally varying microstructural configurations e.g., fiber orientations, fiber volume contents, and fiber length distributions, which render fracture modelling a challenging task. To resolve the microstructure induced anisotropy and its relationship with the macroscopic material behaviour, the well established isotropic phase field models of brittle fracture [1,2,3] is extended towards the anisotropic case making use of the fiber orientation interpolation concept. To create the database, the anisotropic elastic coefficients are obtained from previously executed micromechanical simulations on realistic microstructures using the efficient microscopic solver FeelMath. At the simulation level, the local microstructure must be known in order to access the database: microstructural information stemming from either X-ray micro computed tomography or from injection moulding process simulation is mapped into the Abaqus mesh prior the execution of the macroscopic simulation. The performance of the simulation method is demonstrated by means of several numerical analyses and the prediction quality together with the limitations of the proposed method are demonstrated.

Therefore, an innovative approach is proposed using an offline training of a database plus a fiber interpolation concept to take into account the heterogeneity of the material. The approach is fully integrated into the seamless simulation chain for SFRPs ranging from the manufacturing process to the structure mechanical fracture analysis. The limitations of the approach stemming from the underlying assumptions are quantified and further development needs are identified.

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Solving plane crack problems via enriched holomorphic neural networks

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ABSTRACT

In recent years, there has been a growing interest in leveraging scientific machine learning – a blend of computational methods and advanced machine learning techniques – to solve complex problems in solid mechanics. Particularly, physics-informed neural networks (PINNs) have attracted attention due to their remarkable potential in integrating experimental data and physical models [1].

In the simplest form of the PINN approach, a neural network is used as the ansatz function to solve a boundary value problem. The network weights are optimized during the training stage by minimizing a loss function that includes the residuals of the governing partial differential equations (PDEs), of the boundary conditions (BCs), as well as any deviations from available experimental data [2].

However, a major drawback of the PINN approach is the long training time. In this respect, the recent development of physics-informed *holomorphic* neural networks (PIHNNs) has greatly accelerated the training process for problems where the solution can be represented via holomorphic functions [3]. The reason is that PIHNNs can automatically satisfy the underlying PDEs by enforcing the network output to be holomorphic by construction. Consequently, the goal of the training process reduces to solely finding the network parameters that allow fulfilling the BCs and any available experimental data.

Plane linear elasticity is particularly suited for the PIHNN approach, as the Kolosov-Muskhelishvili representation [4] guarantees that any linear elastic solution can be expressed in terms of two holomorphic functions. On the other hand, a limitation of PIHNNs is their inability to learn discontinuous and singular solutions, as their output, generated by the combination of holomorphic functions, is inherently continuous and smooth everywhere [3]. As a result, the approach is currently unsuitable for problems involving cracks.

To extend the applicability of PIHNNs to crack problems, we investigate in this work the incorporation of enrichment functions in the network representation using two strategies. The first approach, termed Williams-based enrichment, extends the real-valued enrichment introduced in [5] to its complex-valued counterpart. The second approach, referred to as Rice-based enrichment, is a novel strategy uniquely suited to the complex representation of linear elasticity. To demonstrate the potential of the method, stress intensity factors are computed for several case studies, showing superior accuracy and speed compared to the classic PINN approach. Additionally, the efficiency for inverse problems is assessed through a comparison with the Extended Finite Element Method.

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Generating data thanks to digital image correlation results to build models for damage and fracture

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ABSTRACT

In order to build predictive damage and fracture mechanics models, it is necessary to have experimental data on the strain localization and on the crack location. Dense field measurements are a promising lead but analysis of infrared images or global finite element based Digital Image Correlation (without the knowledge of the material behaviour) has limited resolution. In this study, we present a methodology to obtain more accurate local data, in a manner that is independent of material or loading.

First, we use a total variational-like method [1] to obtain, from images of a conventional camera, displacement fields with a better resolution near the crack. Having a satisfactory resolution for full field measurement is important since the local approach to fracture relies on local data.

To exploit local data near the crack, it is necessary to determine the position of the crack. In general, this determination can be divided into two steps. In the first step, one seeks to define the support of the crack path. In this work, an unsupervised learning method (DBSCAN) is used to determine clusters of pixels with high displacement gradients. This enables to select a few pixels corresponding to the strain localization area and to estimate the orientation of the crack with a linear approximation. Local fitting can be performed to better approximate the crack shape. Then, in a second step, empirical criteria are used to determine the position of the crack front along this support. This is done by studying the evolution of a quantity of interest along the support and confronting it with a threshold [2]. An important point is that the value of the threshold should be determined locally. This methodology has been validated by comparison with experimental results obtained with the Direct Current Potential Drop method and with results from another code using Linear Elastic Fracture Mechanics (LEFM) assumptions. However this methodology has also been validated by visual comparison with a blunt crack tip due to large strains. The main interest of this approach is to provide data when LEFM assumptions are no longer valid. The results can thus be used to build damage and fracture models outside the LEFM framework.

In particular, this method also provides data even for very short cracks. In this case, it is proposed to also study the evolution of high displacement gradients in time. We assume that the position of localized strains in the continuum medium can still evolve with time while irreversible phenomena such as damage and crack cannot evolve. This enables us to determine the crack location as well as an area of localized strain in the continuum medium. This last area can be associated with the process zone where local measurements can be made. This method can be used for diagnostics in the context of damage and fracture mechanics. Indeed, it has been applied for fatigue tests on biaxial specimens to determine both the strain localization time and the evolution of the crack length up to a critical value (here 760µm) [3].

In the future, the resulting data could be compared with simulations based on a continuous-discontinuous approach. Optimization procedures can be considered to identify the parameters for the model or for the numerical tools of damage-to-crack transition.

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A hybrid offline-online model order reduction approach for damage propagation problems

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ABSTRACT

To accelerate recursive tasks such as design iterations, computationally efficient methods such as model order reduction are increasingly required. This is because, in structural design, the governing load cases typically involve non-linearities with time and path dependency and makes the models computationally intensive. An example of this problem class is damage modelling. Here, the damage propagation results in a softening response as a function of local stress states which require high dimensional models. Constructing reduced-bases representative of these stress states are intractable since the stress redistribution and the corresponding load paths are difficult to quantify apriori [1]. To overcome this, a hybrid approach involving computations from offline and online phases for reduced-basis and be able to predict damage propagation is developed. In the offline phase, snapshots from only elastic modelling is collected. This offline reduced-basis enables fast computations but limited in accuracy following damage initiation. Therefore, during online phase, reduced-basis in the regions impending damage initiation are updated adaptively with the snapshots collected online. Furthermore, this online reduced-basis is updated recursively consistent with the damage propagation. The reduced-basis is computed with Proper Orthogonal Decomposition (POD) and implemented with Energy-Conserving Mesh Sampling and Weighting (ECSW) hyper-reduction in explicit time integration. This adaptive transformation is performed with minimal disturbance to the surrounding stress state and solution. This method is demonstrated with two open-hole tensile tests of different length-scales and governing damage mechanisms (see Figure 1). In the examples tested, the numerical accuracy and computational efficiency are examined and compared against full-order solutions and experiments.

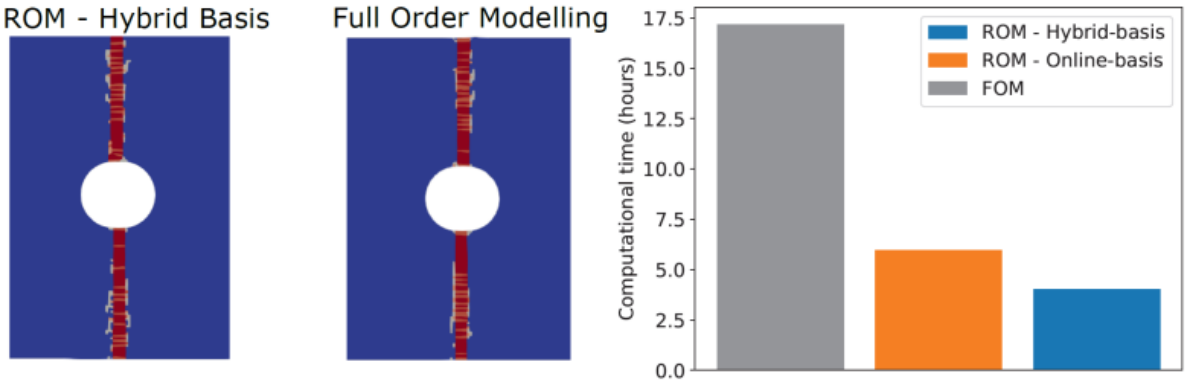

Figure 1 : Comparison of Hybrid and Full Order Modelling

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Influence of Nitrogen Concentration on the Fracture Mechanism of Nitrogen-Doped Gamma-Graphyne Monolayer: A Molecular Dynamics Study

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ABSTRACT

Lithium-air batteries (LABs), with a high theoretical capacity of 3860 $mAhg^{-1}$ and sufficient redox potential (3.04 V vs. standard hydrogen electrode), are considered the next generation and future of lithium-ion batteries (LIBs). This is due to their novel chemical redox reactions, enhanced safety, lower cost, non-toxicity, and approximately nine times higher theoretical capacity compared to traditional LIBs. However, LABs face significant challenges, such as poor cycle life and degradation during charge/discharge cycles, attributed to the loss of coulombic efficiency in the anode and cathode degradation [1].

The cathode, typically constructed from carbon allotropes, can benefit from improved chemical stability through doping processes. Gamma-graphyne [2], a novel carbon allotrope composed of single, triple, and aromatic bonds, shows promise as a material capable of enhancing capacity and gas adsorption sites for LABs. Nevertheless, its chemical resistivity needs to be improved. This enhancement can be achieved by doping nitrogen into the carbon lattice of gamma-graphyne. However, doping can alter the fracture and failure mechanisms of gamma-graphyne, and limited information exists on how these properties vary under different doping levels.

In this context, the current study investigates the effects of nitrogen doping on the fracture mechanism of gamma-graphyne sheets and compares its phenomena with that of the pure material. The results reveal that increasing the percentage of nitrogen doping reduces the mechanical stability of the system and change fatigue crack propagation. Figure 1 illustrates the configurations of pure and 10% nitrogen-doped gamma-graphyne.

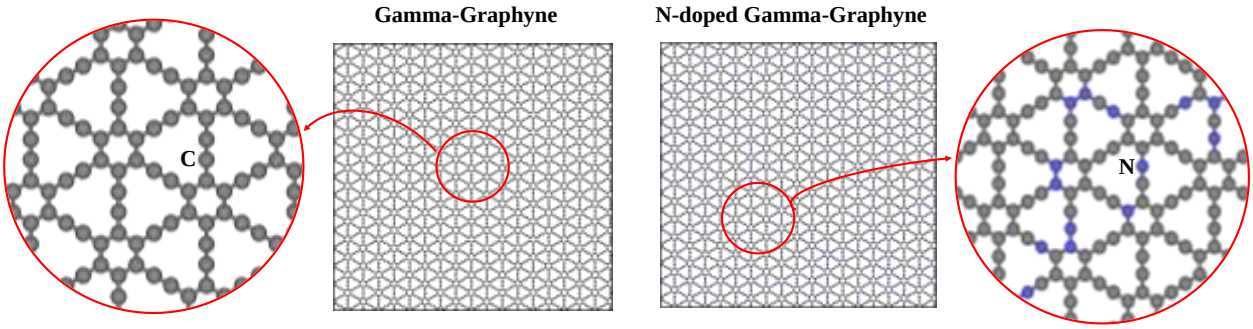

Figure 1 Intercomparison of the configurations of pure and 10% nitrogen-doped gamma-graphyne.

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Uncertainty Quantification in Multiscale Modeling of Composite Materials Using Physically Recurrent Neural Networks

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Keywords: *Multiscale modeling, Machine learning, Composite materials, Uncertainty quantification*

Multiscale modeling of composite materials accurately predicts material behavior but faces high computational costs. To address this issue, neural networks have been used as surrogates for full-order micromodels, predicting their complex behavior accurately. Physically Recurrent Neural Networks (PRNNs) [1] recently demonstrated excellent accuracy for microscale and multiscale simulations with fixed material properties, significantly reducing computational time and requiring minimal training data compared to conventional recurrent neural networks (RNNs). Unlike conventional RNNs, where parameter changes typically require extensive retraining or feature expansion, PRNNs embeds material models in their material layer, which enables modifying material parameters after training.

This study investigates whether a PRNN pretrained on a fixed set of material parameters can maintain accuracy for varying material properties, and thus propagate uncertainty of these properties in a multiscale framework. When material properties are kept fixed during testing, mimicking the rigidity of a conventional RNN, the network loses its accuracy. However, when material properties are adjusted during testing according to the input, PRNN shows high accuracy across a wide range of parameters, accounting for variations in material properties without having to retrain the network.

To evaluate the effect of microscale parameter variations on macroscale responses, multiscale uncertainty quantification (UQ) is performed by comparing full-order and PRNN-driven simulations on an overly coarse mesh. PRNN reduces simulation time by over 7000 times while accurately capturing highly nonlinear force distributions. A PRNN-driven UQ is demonstrated on a more accurate finer mesh, where a full-order UQ would require decades to compute. These results show that otherwise too costly UQ in multiscale modeling of composites becomes possible using PRNNs as an accurate surrogate for full-order micromodels.

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Hybrid neural network for the prediction of damage patterns in composites

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ABSTRACT

Damage pattern predictions of open-hole laminates under different loading conditions are ubiquitous in the finite element modelling of composite structures. The use of machine learning has enabled the fast and accurate surrogate predictions of the performance of composites [1,2]. However, little has been done on the damage pattern predictions using machine learning.

This work investigates the applicability of artificial neural networks for the fast and accurate generation of damage patterns for a composite plate with a cut-out under a variety of loading conditions. Data for training and evaluating these neural networks were generated through nonlinear finite element models. Different neural networks, such as a standard Feedforward Neural Network (FNN) and a Hybrid Neural Network that combines a FNN with a convolutional decoder, have been tested for this task. To quantify the resemblance between the predicted and actual outputs in terms of colours and contours, different performance metrics have been explored. The use of the Structural Similarity Index, in addition to the standard Mean Square Error, was explored to improve the visual quality of outputs from the neural network. The Hybrid Neural Network has been shown to accurately and efficiently predict the damage patterns of the open-hole laminate with small scatter in testing error, thereby constituting a promising candidate for a surrogate model of open-hole composite panels [3].

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Dimensionality reduction of crack tip fields during an overload in fatigue crack propagation

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ABSTRACT

Under service conditions, engineering structures are submitted to complex cycling loading. Fatigue crack propagation is most of the time analysed under an idealized loading condition assuming constant amplitude and constant frequency cycles. A first step to go beyond this ideal case, one can consider an overload cycle. There is no consensus in the literature concerning the impact of an overload on the crack propagation during the following cycles but the most reported effect is an instantaneous acceleration followed by a retardation before the crack goes back to the classical Paris' regime [1].

Before studying the impact of an overload, one has to consider the overload cycle itself. In this contribution, experiments are carried out on SENT specimens made of an aluminium cast alloy. High resolution images are acquired during overload cycles for displacement field computation by digital image correlation. Millions of data (hundreds of images times thousands displacement data) are collected during these cycles. Our approach is based on two steps: first the displacement fields are projected onto the Williams' series [2] and then the obtained crack features (Williams' coefficients like K1, T-stress, B-stress and so on...) are analysed. The latter is carried out trying to reduce the dimensionality of the data to 2: a composite crack feature (a combination of Williams' coefficients) depending linearly upon the applied load and another crack feature that has a non-linear dependency and that activates during the overload phase of the cycle. The analysis is based on singular value decomposition and it ends up, after re multiplying the obtained composite features by the Williams basis functions, with a decomposition of the crack tip displacement field during an overload in a *linear* contribution and a *non-linear* (with respect to the applied load) contribution [3].

A clear separation between these two contributions is obtained. It allows for describing the non-linear processes around the crack tip and their evolution with the applied load by means of only two elementary displacement fields and their respective amplitude. We further show that the amplitude of the *non-linear* field depends on the intensity of the *linear* field following a unique relation. This relationship can be interpreted as a crack tip constitutive relation which could be fitted with a phenomenological description to be incorporated in a crack propagation model accounting for the effects over overloads.

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Fracture in concrete: X-ray tomography with in-situ testing, digital volume correlation and phase-field modeling – CFRAC 2025

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ABSTRACT

The complex crack nucleation and propagation behavior in concrete is largely influenced by its mesostructural arrangement, thus, it is important to account for it to obtain realistic predictions of concrete fracture [1,2].

X-ray computed tomography (CT) can be adopted not only to obtain the real 3D mesoscopic geometries [2], but also to visualize the crack onset and the 3D complex crack propagation pattern during a mechanical test [1,3]. This information can be obtained from in-situ testing, i.e. by carrying out a mechanical test inside the tomograph and taking several CT images of the sample at different stages of the test. Moreover, using digital volume correlation (DVC) it is possible to measure the 3D displacement field [1,3].

The aim of this work is to complement finite element computations based on the phase field fracture model with experimental data including CT and DVC measurements to reproduce the concrete cracking behavior at the mesoscale, namely, explicitly resolving aggregates and pores in the geometry. To this end, experimental tests are performed to characterize elastic and fracture parameters of both mortar and aggregates. Then, a series of in-situ wedge splitting tests is performed on concrete specimens doped with baryte contrast enhancers to improve phases segmentation [2]. The CT image of the specimen before loading delivers the real mesoscopic 3D geometry, while from DVC analysis on the time series of images we obtain the 3D full-field displacement data including realistic boundary conditions that can be adopted in the numerical simulations. Finally, we perform numerical simulations on the real geometry with the real boundary conditions and compare numerical and experimental results.

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Automated characterization of CFRP crack propagation

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ABSTRACT

Digital Image Correlation (DIC) [1] is a non-contact, full-field optical measurement technique that has found significant applications in assessing material deformation and crack propagation. The utilization of DIC data as input for numerical simulations, such as Finite Element Models (FEM), can improve the accuracy and reliability of crack growth predictions, making it a valuable tool to make virtual testing and optimization credible.

This paper discusses the methodology of integrating DIC measurements with numerical models and outlines its application to crack measurement in the case of interlaminar crack propagation testing of laminate composite materials.

The work performed in this study uses only the DCB (Double Cantilever Beam) test, which is regularly chosen in research work because it is characterized by the fact that it supposedly stresses only mode I. Safran Aircraft Engines expressed its will to improve its DCB test procedure by automating the crack length measurement for each test by using "global" image correlation. In this technique, the user can perform an alignment between the measurement mesh and the reference image after importing the test images and selecting the measurement mesh.

Following the crack tip from the displacement field, once the study is completed, the use of "global" DIC [2] makes it possible to export the displacement and strain results at the nodal locations. This functionality is particularly useful in this project to determine the crack advance during the DCB test. The solution developed here is a Python post-processing script designed to determine the crack length along the DCB test by exploiting the data exported from DIC.

In conclusion, digital image correlation offers a robust and efficient method for monitoring crack propagation in materials. Its integration with numerical simulations enhances the predictive capabilities of structural analyses, leading to more accurate assessments of material performance under stress. By incorporating real-world measurement data from DIC, simulation results can be adjusted to reflect true material behavior under load, facilitating a deeper understanding of failure mechanisms. Furthermore, DIC can serve as a benchmark for validating numerical models, ensuring that the simulations align closely with experimental findings.

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Meta-neural Topology Optimization

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ABSTRACT

Engineers learn from every design they create, building intuition that helps them quickly identify promising solutions for new problems. Topology optimization (TO) is a well-established computational method for designing structures with optimized performance but lacks this ability to learn from experience. Existing approaches treat design tasks in isolation, starting from a "blank canvas" design for each new problem and often requiring many computationally expensive steps to converge. We propose a meta-learning strategy, termed meta-neural TO, that finds effective initial designs through systematic transfer of knowledge between related tasks, building on the mesh-agnostic representation provided by neural reparameterization. We compare our approach against established TO methods, demonstrating faster convergence without compromising the final design quality. Further, we demonstrate cross-resolution transfer, where initializations learned on lower-resolution tasks lead to superior convergence in 74.1% of tasks from a higher-resolution test set. Remarkably, we discover that meta-learning naturally gravitates toward strain energy field patterns as effective initial designs, aligning with engineering intuition for compliance optimization problems.

Mesh cutting and compile-time many-to-many relation framework for adaptive remeshing in computational fracture

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ABSTRACT

In this paper, we introduce two new open-source libraries. The first is a library to carry out edge cut based remeshing on a simplicial 3-complex. The result is concise, performant (more than 130 million tetrahedra are cut in less than one minute in a traditional laptop) and can be used for most remeshing tasks related to crack propagation. Six verification examples are presented, that illustrate the use of the library. The second is a many-to-many dependence manager based on compile-time schema, compile-time reflection (Boost PFR) and type list manipulations. This is able to i) perform serialization tasks automatically, ii) dynamically modify entities in any discretization framework, iii) perform relationship queries based on symbolic sparse linear algebra. For example, a symbolic assembling process is a multiplication of incidence tables, which are also type incidence tables: $(EL.N \times N.DOF)^T \times (EL.N \times N.DOF) + \cdots + (EL.EDGE \times EDGE.DOF)^T \times (EL.EDGE \times EDGE.DOF)$. A compile-time object factory is established, with schema for child objects being invoked during object creation. I.e., a new tetrahedra automatically registers edges and faces in the existing mesh. A heterogenous container is established using the typelist library and both registration and retrieval are achieved using template parameters.

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Estimation of Fatigue Crack Propagation in FSW Joints Using SVR

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ABSTRACT

To predict the crack growth life of friction stir welding (FSW) structures efficiently and accurately, a fatigue crack propagation life prediction method based on support vector regression (SVR) for 2195 Al-Li alloy FSW joints is proposed. First, the Paris crack growth model constants and crack tip stress intensity factor dataset were obtained through fatigue crack growth testing and finite element simulation. Next, a stress intensity factor prediction model based on the SVR model is developed, and its hyperparameters are optimized using the particle swarm optimization (PSO) algorithm. Finally, crack propagation life is predicted using the stress intensity factor prediction model and the Paris model. The results demonstrate that the optimized PSO-SVR model can predict the crack tip stress intensity factor efficiently and accurately, with the coefficient of determination (R^2) on the test set reaching 0.9995, which is higher than the 0.954 achieved by the unoptimized SVR model. The predicted crack growth life is compared with the results from finite element simulation. The maximum error is less than 5%, confirming the accuracy of the method.

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Minisymposium DMMF:

Discrete models for material failure

Organized by F. Kun, F. Wittel, J. Eliáš and G. Cusatis

Dynamic tensile concrete behaviour – effects of free water and aggregate fragmentation using a coupled DEM-CFD approach

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ABSTRACT

This study investigates the effects of free water and aggregate fragmentation on the dynamic behavior of concrete under uniaxial tension [1]. Concrete was simulated as a four-phase material consisting of aggregate, mortar, ITZs, and macropores. The concrete mesostructure was obtained from laboratory micro-CT tests.

A novel fully coupled DEM/CFD technique, based on a pore-scale hydro-mechanical model [1]-[3] was used to predict the effect of free water on the response of both partially and fully fluid-saturated concrete. The method's concept was creating a network of channels between discrete elements in a continuous space to produce a flowing movement. Partly saturated concrete with minimal porosity was suggested to have a two-phase laminar fluid flow (air and water). To accurately track the liquid/gas content, the position and volumes of the pores and cracks were considered. A so-called clump breakage algorithm [4] was applied to imitate intra-granular fragmentation of aggregates. Clumps composed of small spheres were used to describe the aggregate particles of different diameters and shapes. Different aggregate strengths were assumed. Numerical analyses were performed using YADE, a 3D open-source DEM program that takes advantage of the so-called soft-particle approach (i.e. the DEM model allows for particle deformation that is simulated as an overlap of particles).

Attention was paid to the strength, brittleness, fracture patterns, and free water pressures and velocities in concrete specimens under different strain rates, changing between 0.1 1/s and 100 1/s. The numerical DEM-CFD results matched the corresponding findings of the laboratory tests, based on split Hopkinson pressure bar (SHPB) tests.

The compressibility of fluid phases affected the dynamic compressive strength more than viscous fluid flow in contrast to the quasi-static tests [2]. The free water migration and aggregate fragmentation increased the dynamic impact factor (DIF).

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Controlling fragmentation dynamics of exploding rings in a two-dimensional discrete element model

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ABSTRACT

Energetic loading, such as impacts or explosions, causes solid bodies to rapidly disintegrate into numerous pieces with diverse shapes and sizes [1]. These dynamic breakup processes are widespread in nature, manifesting in events like volcanic pyroclastic activity, rock wall collapses, and glacier breakups within our geological environment. A key challenge in fragmentation research lies in accurately predicting and controlling the size (mass) distribution of the resulting fragments [2].

We present a computational study on the fragmentation dynamics of brittle, heterogeneous rings subjected to explosive loading, conducted using a two-dimensional discrete element model (DEM). In our DEM, rings are discretized on a random lattice of convex polygons, which are connected by elastic breakable beams. Our simulations reveal a sequence of transitions between distinct fragmentation regimes as a function of strain rate and ring thickness. At low strain rates, fragmentation occurs via radial segmentation, producing fragments with Weibull-type mass distributions. As strain rates increase, planar fragmentation emerges, characterized by power-law distributed masses. At the highest strain rates, complete shattering of the ring is observed.

Critical strain rates marking the transitions between segmentation, planar fragmentation, and shattering were identified. Notably, the crossover regime between one-dimensional and two-dimensional fragmentation processes provides a controllable parameter space for tailoring fragment mass distributions. By adjusting strain rate and ring thickness up to a critical value, the mass distribution exponent can be systematically modified. These insights are particularly valuable for applications requiring precise control over fragmentation outcomes, such as space debris management [3] and defence technologies [4].

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Discrete element model for the anisotropic cracking of shrinking material layers

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ABSTRACT

Mechanical perturbation of thin layers of pastes on a substrate results in anisotropic cracking during desiccation which allows for a controlled generation of crack patterns with a high relevance for industrial applications [1].

To study shrinkage induced cracking, discrete element modelling (DEM) provides an adequate framework being able to capture the details of materials heterogeneity, furthermore, the dynamics of deformation and crack formation [2,3,4]. Here we propose a DEM to capture the anisotropy induced by initial perturbations which imprint directional dependent material features into the layer. Our approach is based on a random tessellation of the layer using convex polygons which are made anisotropic by elongating or compressing them along the direction of perturbation [3]. Physical properties of the particles' cohesive contacts are determined by the geometrical characteristics of polygons giving rise to a well controlled anisotropy in the mechanical response of the material and in the structure of the fracture pattern emerging during shrinking. The main advantage of the approach is that both the structural disorder of the layer and the strength of anisotropy are controlled by a single parameter. Based on computer simulations we demonstrate that varying its two parameters the model reproduces the qualitative features of experimental findings and provides advantages over existing modelling approaches [3].

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A novel DEM-based coupled 3D thermo-hydro-mechanical mesoscopic model with phase changes for concrete shrinkage modeling

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ABSTRACT

The moisture content and ambient humidity strongly influence concrete shrinkage. The effect of the humidity is currently considered in models and design codes by time-average considerations, thus totally neglecting cyclic changes in ambient humidity normally observed in outdoor structures. The influence of the cyclic ambient humidity on the long-term deformations of concrete compared to the constant mean humidity was, however, rarely investigated.

A novel DEM-based pore-scale 3D thermo-hydro-mechanical (THM) model of two-phase fluid flow and heat transfer in fluid and solids was used to study a process of concrete shrinkage [1]. The model is based on a direct numerical simulation approach. The model's original concept is based on the notion that in a physical system, two domains coexist: the 3D discrete (solid) domain and the 3D continuous (fluid) domain [1]. Both domains are discretized into a coarse mesh of tetrahedra. The model [1] considers now phase changes in the fluid.

The THM model was validated by comparing the numerical results with the analytical solution of the classic 1D heat transfer problem. Numerical calculations were carried out for bonded granular specimens imitating concrete with a 3D DEM fully coupled with 3D CFD (based on a fluid flow network) and 3D heat transfer that linked discrete mechanics with fluid mechanics and heat transfer at the mesoscale. The heat transfer was related to the fluid (diffusion and advection), bonded granular particles (conduction), and phase changes.

Perfect accordance was obtained between numerical and analytical outcomes. Moreover, the influence of phase changes in the fluid on heat and mass transfer in the bonded particle assemblies and its deformation was numerically presented. The numerical outcomes of concrete shrinkage were directly compared with corresponding experiments in the literature.

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Predicting fracture in 3D printed concrete lattice systems with the QuasiContinuum method

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Abstract

3D-printed concrete (3DPC) mitigates CO_2 emissions, provides architectural design with higher degrees of freedom and decreases both labor costs and energy consumption. However, its layer-by-layer build-up process results in weaker and more porous interlayers, thereby significantly decreasing the integrity and durability of 3DPC structures and limiting the versatility of this technology. The porosity is characterized by elongated air voids aligned with the printing direction, leading to stress concentrations and reducing the interlayer bond strength [1].

Lattice systems are indispensable for modeling and analyzing physical phenomena in materials with heterogeneous micro- or meso-structures such as 3DPC. However, the computational requirements for practical engineering applications of lattice systems remain high. The QuasiContinuum (QC) method addresses this by reducing the system of equations using a finite element mesh with linear interpolation. Instead of considering all Degrees of Freedom (DOF), the QC method reduces the system of equations by interpolating the displacement of lattice nodes based on a coarser triangulation in regions of low interest. The multiscale characteristics of QC enable a seamless transition to a fully-resolved lattice at locations where damage and fracture occurs [2]. Nevertheless, interfaces between separate phases in heterogeneous materials, such as 3DPC, require fine meshes throughout the domain, diminishing the effectiveness of QC. Enrichment strategies of the eXtended Finite Element Method (XFEM) can account for material interfaces using nonconforming meshes, resolving this issue. In a previous study, we applied Heaviside enrichment to investigate concrete meso-structures with the QC method, achieving a tenfold reduction in the number of unknowns while maintaining similar accuracy compared to discretizations with fully resolved interfaces [3].

In the present study, the micro-structure of 3DPC is modeled by a regular discrete lattice based on a truncated octahedron unit cell with truss elements. The air void morphology in the interlayer region is accurately represented by enrichment methods of the XFEM. This allows for the consideration of stress concentrations resulting from the air voids on the interlayer bond strength. Numerical 3DPC samples are studied under flexural loading up to their load limit. A quasi-brittle fracture criterion is applied to the lattice members, and an element is deactivated when a maximum stress threshold is reached and a crack initiated.

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Numerical analysis of cracking behavior and ultrasonic wave propagation in reinforce concrete for damage classification using DEM and FDM

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ABSTRACT

Effective crack control in reinforced concrete is essential to prevent steel corrosion and maintain the structural durability of critical infrastructure. However, given ever-increasing traffic demand, the current inspection methods, including annual routine checks and six-year comprehensive reviews, are labor-intensive and insufficient for aging infrastructure. Ultrasonic monitoring with coda wave interferometry (CWI) [1] offers a promising and cost-effective approach for detecting subtle structural changes beyond the limits of standard inspection techniques.

In this regard, understanding damage progression at various stages of deterioration in reinforced concrete is crucial for reliably interpreting and correlating wave features, such as relative velocity changes, with the corresponding levels of structural damage. To this end, this study proposes a computational framework to complement experimental investigations and generate synthetic datasets for crack monitoring using advanced statistical and machine learning methods. The framework integrates the Discrete Element Method (DEM) to model damage behavior of reinforced concrete under tensile loads and the Finite Difference Method (FDM) to simulate wave propagation in cracked concrete. A realistic numerically generated concrete mesostructure [2], including aggregates, steel reinforcement, and their interactions, is explicitly modeled. Numerical results are validated against experimental measurements, and mechanisms affecting wave variantions are analyzed. Finally, a strategy for fusing synthetic and experimental data to classify damage stages is proposed and discussed.

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Minisymposium DF:

Ductile fracture

Organized by P.O. Bouchard, J. César de Sá and R. Peerlings

Calibration and Validation of Ductile Failure Models for a Plate Puncture Experiment

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ABSTRACT

The puncture of metallic components represents an important problem in structural mechanics, with diverse applications such as vehicle-impact safety analyses and armor design. Colleagues at Sandia National Laboratories have recently developed a puncture challenge problem, following the series of Sandia Fracture Challenges, featuring drops tests of increasing height until an aluminum 6061-T6 target is punctured. Extensive characterization testing of the base material was performed.

In this presentation, we propose forms for a ductile failure model meant to respond to this challenge. We propose a multi-step model calibration procedure, beginning with a base plasticity model, then extending with the failure model. Proposed plasticity models include J_2 (von Mises) Hill yield surfaces with rate- and temperature-dependence options; damage models include a stress-state dependent Wilkins damage model [1] and a micromechanical Bammann-Chiesa-Johnson damage model [2]. We document the calibration process and perform validation of the model on the puncture challenge problem and discuss remaining gaps with the failure models, including the role of anisotropy.

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3D transition from continuum ductile damage models to discontinuous crack propagation within the context of material forming

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ABSTRACT

In the context of material forming, predicting and preventing the onset of possible crack initiation is of outmost importance to ensure final components quality and properties. There is a huge scientific literature devoted to ductile damage analysis in material forming [1] with approaches either based on uncoupled ductile fracture criteria or coupled damage models. However, in specific cases, predicting the onset of crack initiation is not enough and modeling the subsequent fracture initiation and propagation is also necessary. This is for example the case for multi-stages forming processes that include blanking and cutting processes. In these configurations, the quality of the fracture surface obtained after blanking is important to address possible failure initiation on these new free surfaces in the following forming operations. For such applications, the use of the kill-element technique, even improved with mesh adaption or smoothing techniques [2], may not be accurate enough.

In order to address such applications, this work presents a methodology that enables a smooth transition from continuum damage mechanics to discontinuous 3D crack propagation. A phase field model, adapted to ductile damage, is implemented in the finite element software Forge®. The crack initiation and insertion in the 3D mesh is handled through the use of an efficient strategy using both accurate description of the phase field gradient and mesh adaption [3, 4]. This methodology is confronted to various metal forming applications [5, 6] and its accuracy and efficiency is discussed.

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Third-invariant effects on damage and fracture of isotropic materials

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ABSTRACT

This paper is devoted to the investigation of the role played by the third invariant of the stress deviator, J_3 on damage evolution and fracture of ductile isotropic materials. For both compressive and tensile loadings, finite-element **(**FE**)** unit-cell simulations were conducted at fixed stress triaxialities and various ordering of the principal stresses. The matrix material was described using the isotropic yield criterion of Cazacu (2018). This yield criterion involves a unique parameter, a; in the case when a=0 it reduces to the von Mises yield criterion while for a different from zero, it has dependence on J_3. F.E. unit cell model simulations for materials characterized by various values of the parameter α put into evidence the role played by the particularities of the plastic deformation on damage evolution. A new homogenized potential is introduced. This potential captures all the trends shown by the unit cell simulations and enables us to explain fracture characteristics under shear loadings put into evidence experimentally.

A hybrid micro-mechanics based and data-driven ductile fracture model

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ABSTRACT

Trustworthy knowledge of damage evolution and fracture of materials is crucial in design of safe and sustainable structures. With proper calibration, the analytical framework for plastic strain localisation presented by Rice [1] has been shown to provide realistic predictions of ductile fracture initiation. Previous work by the authors has shown that this framework is well suited for calibration of ductile fracture models [2] and as a post-processor step to predict ductile failure initiation [3].

For the predefined load histories observed in pre- and post-processing steps, strain localisation analysis has proven very efficient. However, in finite element simulations, the stress state in one element will not only vary with time, but also mutually depend on the response in other parts of the finite element model. This implies that localisation analyses across many imperfection bands must be carried out for all integration points in a finite element mesh and at all time steps to be sure to capture the most critical band. Hence, an excessive number of computations, as well as data storage, would be necessary to carry out strain localisation analyses in-situ finite element simulations.

To avoid this issue, we study how knowledge on existing ductile failure modelling can be combined with machine learning methods using data from strain localisation analyses to establish a surrogate hybrid ductile fracture model. The artificial neural network part of this surrogate model is trained using data from strain localisation analyses, while the analytical part of the model ensures well-known properties of micro-mechanical behaviour. The study shows that combining conventional fracture models with machine learning approaches has a potential within ductile fracture modelling.

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Phase field modelling of ductile damage: application to underwater explosions of hull structures

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ABSTRACT

In the context of material qualification for naval structures, various strategies are employed to evaluate the structural response to underwater explosions. One such approach is the Bulge Explosion Test (BET), which makes it possible to test the capacity of hull steels to withstand significant deformation without failure. Numerical simulation of a BET enables assessing residual and damage states of hull steels at every stage of an underwater explosion. This requires that the implemented laws accurately describe the material's failure behavior and that the parameters of these laws are correctly identified.

The present work will discuss the ability of the phase field approach to describe the failure behavior of hull steels within the finite element software ABAQUS®. The phase field method is on the rise and has already been widely used in the context of brittle fracture [1]. It offers the advantage of an accurate crack localization compared to conventional non-local formulations. Different extensions were proposed to address ductile failure [2,3]. In this paper, we propose a formulation based on the work of [2], which incorporates a dependency of the phase field on the stress states [4], along with additional parameters that require calibration.

A phase field model has therefore been developed to investigate the ductile response of a thick plate subjected to dynamic loadings. The model is compared to the Lemaître damage model, regularized with an implicit gradient non-local formulation. Both models were calibrated based on experimental specimen exhibiting a large range of stress triaxiality ratio and Lode parameter: smooth and notched round bars, flat-grooved and mini-punch specimen.

To assess the ability of the two models to describe the failure behavior of hull steels under BET, experimental and numerical tests were conducted on thick steel plates subjected to single and multiple BETs. Experimental tensile specimen are machined from deformed steel plates and comparisons are carried out between experimental results and numerical predictions.

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Revisiting ductile fracture with random porous metamaterials

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ABSTRACT

Ductile fracture is a common failure mechanism of metals and alloys. It consists of several stages, which involve the nucleation, growth and coalescence of microscopic voids within the metallic matrix. These mechanisms are driven by plastic deformation and their quantification is essential to develop physics-based predictive models of the ductile fracture process.

In this work, X-Ray tomography is combined with full-field kinematic measurements in order to probe the mechanisms of void growth and coalescence at the mesoscale. To this end, a novel class of model materials is designed, which is referred to as *random porous metamaterials* and contain random distributions of cylindrical pores, embedded within a ductile metallic matrix. The pores have arbitrary elliptical shape and micrometric size, and are precisely engineered from design to manufacturing. Their arrangement and geometry are generated by means of a random sequential absorption algorithm and are fabricated by laser powder-bed fusion (LPBF) [2].

Using FE-based Digital Volume Correlation (DVC) with mesoscale meshes consistent with the pore distribution, the mechanisms of void growth and coalescence (during tensile straining) are quantified for this class of cellular solids. It is shown that highly heterogeneous deformation patterns result from the random pore arrangement and delay long-wavelength strained bands. The measured data for the pore strains are highly scattered, and exhibit a departure from McClintock's model predictions for the voids within the fracture band.

The experimental findindgs are rationalized on account of the interaction between the cylindrical voids. The latter increases with higher pore aspect ratio, and is, in turn, promoted by the presence of defects forming inevitably during manufacturing. Two types of process-induced defects (i.e. small pores and irregular cracks) are distinguished using X-Ray tomography, and are shown to contribute differently to the fracture process. To investigate their influence on the observed strain patterns, a Finite Element Model Updating (FEMU) technique [3] is implemented using locally-damaged meshes, in which pre-existing defects are first identified (from the initial tomography) and removed from the nominal (defect-free) mesh.

Collectively, this study highlights the potential offered by random porous metamaterials, which can be harnessed to revisit the complex mechanisms of ductile fracture at the mesoscale.

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Strain Hardening Effect on Ductile Crack Propagation under Small-Scale Yielding Plane Strain Conditions

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ABSTRACT

The influence of strain hardening on ductile crack growth is analyzed using a small-scale yielding finite element approach under plane strain conditions. This study relies both on J2 plasticity and on an advanced nonlocal Gurson model [1]. Strain hardening exponents n up to 0.5 are investigated, extending our focus beyond classical studies to include materials such as stainless steels, TRIP-TWIP alloys, and high entropy alloys. The J2 plasticity simulations reveal how higher values of n reduce the extension of the finite strain zone and modify the distribution of opening stress and the crack tip opening displacement. This provides indirect insights into how strain hardening impacts fracture toughness. Additionally, Gurson-based simulations are performed under a nonlocal formulation with varying levels of strain hardening and initial porosity, generating JR curves, tearing modulus, and crack initiation metrics, such as JIC and critical crack tip opening displacement. These simulations demonstrate that fracture toughness increases with higher values of n. The following questions are addressed: (i) Why does fracture toughness increase with n? (ii) How does a very high n affect fracture resistance indicators? (iii) What is the potential impact of developing metallic alloys with a high strain hardening capacity? Furthermore, we emphasize the need to fine-tune the Gurson model for high strain hardening exponents and to establish precise guidelines for mesh generation and initial crack opening to ensure accurate results.

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Global versus local ductility in two-phase microstructures

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ABSTRACT

Advanced engineering materials often have microstructures which consist of multiple phases or base materials. The purpose of such material designs generally is to pair a high strength with a high degree of deformability – where the former stems from strong, but often brittle, particles and the latter from a comparatively soft but ductile matrix. Failure of such materials may on the one hand be introduced by necking – a geometrical instability – or on the other by the nucleation and growth of damage – i.e. material instability. The former is sometimes referred to as global ductility and the latter to local ductility. Experiments tend to show that these properties are competing, i.e. microstructures which have an excellent global ductility turn out to have a poor local ductility, and vice versa. In this study we investigate the origin of this paradox. We approach the problem at an abstract level, using a highly idealised two-dimensional model which includes only the key features of the microstructure. The model assumes the phases to be randomly distributed in a square grid and defines two competing failure mechanisms – one for each phase. Its simplicity greatly facilitates the interpretation of results and allows one to run many (hundreds of) simulations, thus enabling a wide range of parameter variations. Despite its simplicity, the model captures, and helps to explain, the above paradox [1]. Additional questions which the model helps to answer are how pre-existing defects affect strength and ductility and how the formability depends on stress state – in particular on stress triaxiality and Lode angle [2].

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Experimental Assessment of the Mechanical Properties of API Steel Under Hydrogen Embrittlement for Repurposing Natural Gas Pipeline Networks

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Abstract:

This study presents an experimental evaluation of the mechanical properties of API 5L Grade B steel subjected to hydrogen embrittlement (HE) to assess its suitability for repurposing natural gas pipelines for hydrogen transportation. Hydrogen embrittlement is a critical issue for metallic materials, as hydrogen diffusion into steel can significantly degrade its mechanical properties. Tensile tests, crack propagation tests, and fracture toughness evaluations were conducted on specimens extracted from in-service pipelines, exposed to hydrogen under simulated operating conditions at pressures up to 100 MPa with varying hydrogen-methane mixtures (e.g., 100% H_2 and 20% H_2 + 80% CH_4). The results reveal that while the tensile strength of the material remains largely unaffected by hydrogen, its ductility and fracture toughness are significantly reduced. Crack propagation rates increase in hydrogen environments, raising concerns about potential brittle fractures and accelerated failure mechanisms. Despite the negative effects of hydrogen, the fatigue crack growth rates were still within the acceptable limits set by the ASME B31.12 code, suggesting that API 5L Grade B steel remains viable for hydrogen service with appropriate safety measures. This study highlights the need for rigorous pipeline integrity monitoring and suggests further research on material modifications to enhance hydrogen resistance, supporting the ongoing energy transition toward hydrogen as a clean fuel.

Keywords: Hydrogen embrittlement; API Steel; Hydrogen transportation; Crack propagation; Fracture Toughness.

Minisymposium DFMS:

Dynamic fracture of materials and structures

Organized by M. Jabareen and P. Areias

Ductile fracture modelling using the Extended Finite Element Method for dynamic analysis

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ABSTRACT

An extension of the three-dimensional numerical methodology proposed by [1] is presented with the aim of reproducing the different phases of ductile fracture in the context of transient dynamics while considering large deformations, high strain rates and high temperatures. Simulations are conducted using the extended finite element method (XFEM) with both implicit and explicit integration schemes. A lumping technique of the enriched mass matrix is also proposed.

The material considered in this work is supposed to obey the GTN micro-porous plasticity model [2]. Its hardening is of the form of a Voce type law. As usually done, the ductile fracture is considered a 3-phase process: (i) diffuse damage by nucleation and growth of voids, (ii) strain localization and (iii) propagation of a macro-crack. Strain localization process is tentatively neglected. Indeed, a direct transition between diffuse damage and crack propagation is considered, case similar to the ductile fracture criterion proposed by [3]. The numerical treatment of the crack is achieved by using the extended finite element method (XFEM). As it is generally done in dynamics, the mass matrix is diagonalized primarily to increase the stable time increment [4]. A mass lumping technique in the context of the shifted basis of the XFEM [5] is presented and a particular attention is paid to the kinetic energy conservation [6].

The model developed by [1] and extended to solve dynamic problems was implemented in an Abaqus user element for both implicit and explicit resolution. Dynamic tests on CT specimens were carried out and the results obtained with each time integration scheme were compared in term of stiffness evolution, porosity profile, crack progression and energy balance.

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The Application of the SPH and the Adaptive FEM-SPH Techniques for Modeling of Damage and Failure of Satellite Shielding Under Orbital Debris Impact

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ABSTRACT

Spacecraft must be analyzed for their ability to survive hypervelocity impacts (HVI) by orbital debris, as the collision of a space vehicle with even a millimeter-sized object traveling at a typical orbital speed (7 km/s and higher) can be detrimental for both the spacecraft and the orbital environment. Due to the high cost of the physical HVI experiments, numerical modeling plays a significant role in conducting such analyses.

This presentation will discuss the modeling of spacecraft shielding, comprised of sandwich panels with honeycomb- or open-cell foam cores, subjected to hypervelocity impact by orbital debris. The simulations employed a combination of the smoothed particles hydrodynamics (SPH) and the adaptive FEM-SPH technique for the representation of hypervelocity projectiles and different components of the shielding systems.

In particular, for *honeycomb-core panels*, the front facesheets were modeled using SPH particles, while the rear facesheets' representation employed the adaptive FEM-SPH technique, in which finite elements could locally and adaptively transform to SPH particles when the elements become highly distorted and inefficient.

For *foam-core panels*, both facesheets were modeled using the adaptive method, while the foam core itself featured an explicit and realistic representation of its complex mesoscopic architecture. This was achieved by filling the STL exteriors (generated using X-ray computed tomography) with SPH particles, making it suitable for HVI simulations.

The capability of the developed simulation models to predict damage and failure of the shielding systems under hypervelocity impact was evaluated by comparison with data from NASA and ESA experiments.

Stabilization of Extrinsic Cohesive Elements in Explicit Dynamic Fragmentation Simulations

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Abstract

The increasing density of satellites and debris in Low Earth Orbit (LEO) heightens the risk of hypervelocity collisions. During such high-energy events, the involved structures undergo rapid and catastrophic failure, a process known as dynamic fragmentation. This phenomenon is of significant concern in the aerospace industry which requires accurate and scalable models to predict the resulting fragment statistics. To address this, the presented numerical work leverages the Cohesive Zone Model (CZM), with extrinsic cohesive elements, using the explicit dynamic time integration scheme, based on Newmark-β. The model is coupled to a penalty-based approach for contact and friction, and benefits from a parallel implementation [1].

The initiation and propagation of numerous cracks, repeated contacts and friction among crack faces and moving debris particles result in a non-smooth behavior, characteristic of dynamic fragmentation. Although the chosen explicit approach is scalable, it inherently introduces instabilities that can compromise the accuracy of fragment statistics [2]. To address this, an innovative stabilization strategy is proposed, focusing on maintaining a stable energy balance throughout the simulation. This strategy addresses instabilities caused by the excessive initial cohesive stiffness upon the insertion of new cohesive elements, as well as from nonlinearities during contact and softening regimes. Locally, at a cohesive element, as the damage variable d approaches zero – where cohesive stiffness, inversely proportional to damage, tends toward infinity – a viscous term is added to the cohesive traction to stabilize crack opening. Additionally, when contact or softening is detected, a velocity-based stabilization method is applied. To ensure global energy balance, the local kinetic energy of bulk elements associated with the unstable cohesive element is adjusted to offset spurious energy variations.

Key results of dynamic fragmentation simulations include the fragment count and the distribution of mass and velocities. From such outputs, we validate our model against a robust, computationally intensive LCP-based implementation of the problem, maintaining discrete energy balance [3]. The results demonstrate our model's capability to extend to larger, more confined systems, subjected to fracture, unilateral contact, and friction.

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Dynamic fracture of thin incompressible membranes at finite deformations

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ABSTRACT

In the present study, a finite element formulation for modeling crack propagation in hyperelastic thin membranes is developed. The crack formation and propagation are modeled by means of the material-sink approach stemming from the physical observation of the diffused bond breakage. Keeping in mind that loss of local bonds leads to localized material loss, the mass density can be considered as a variable, which numerically decreases in the area where damage localizes into a crack. This notion requires mathematical consideration of mass balance as an additional and active law, which regularizes the computational model. From the numerical point of view, the developed computational model has displacement and density degrees of freedom. Also, a monolithic approach was applied that ensures stable incrimination of the nonlinear problem. Numerical examples of the fracture of different geometries demonstrate the high robustness of the proposed approach in modeling crack propagation in membrane structures.

A bond-associated peridynamic approach to fracture in thin structures

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Peridynamics is a nonlocal continuum mechanics approach widely used for modeling damage and fracture phenomena. There are different formulations of the underlying theory to realize the same material behaviors as observed in reality and described by the classical (elastic) theory. In particular for thin structures, the non-locality induces surface effects. The correspondence formulation of peridynamics mitigates these limitations, utilizing an approximated deformation gradient to calculate stress forces. Although this reformulation improves the accuracy of elastic modeling, it introduces instabilities. These problems combined make it hard to model dynamic fracture with large deformations in thin structures.

This contribution presents a comprehensive review of bond-associated peridynamic formulations as a promising solution to these challenges. Various approaches within bond-associated modeling are compared, focusing on computational efficiency and other factors regarding discretization and computational implementation.

The analysis confirms that bond-associated models effectively capture the correct fragmentation process in thin structures. Explanatory examples of dynamic fracture in thin structures are provided, showcasing the capabilities and practical relevance of these models.

Keywords:
peridynamics, dynamic fracture, thin structures, bond-associated peridynamics

Comparison of XFEM and phase field method for fracture simulation of two-dimensional asymmetrically bent plates with holes

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ABSTRACT

Fracture is one of the main forms of failure of engineering materials, and accurate simulation of the crack extension process has important engineering value, and a variety of research methods exist. The extended finite element method (XFEM) uses an expanded form function basis to represent discontinuities, and the simulated discontinuous displacement field is completely independent of the mesh boundary without the need for re-meshing; the phase field method uses a diffuse phase field to describe the smooth transition between the unbroken and broken material, and can deal with different types of fracture in a unified framework. The two methods are computationally efficient with good solution convergence, and can achieve automatic tracking of crack extension, which have unique advantages in the solution of complex fracture problems. In order to explore the performance differences between the two types of methods in detail, this paper applies the commercial finite element code Abaqus/Standard to establish brittle fracture models based on XFEM and robust staggered phase field solution, respectively, and conducts the crack extension analysis on a two-dimensional perforated asymmetric bending plate, and compares and analyses relevant numerical calculations with experimental results. The results show that both XFEM and phase field method can automatically predict the crack extension path of 2D asymmetric curved plate with holes, and the extension path is not affected by the finite element mesh boundary. However, the results of the phase-field method are closer to the experimental results as the cracks get closer to the holes, which suggests a higher accuracy of the phase-field method.

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Supershear growth of tensile cracks enabled by geometric non-linearities

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The theory of Linear Elastic Fracture Mechanics (LEFM) asserts that a crack's propagation speed is limited by the Rayleigh wave speed. Many experimental and numerical studies have aligned with this theory; however, some exceptions raise questions about its validity and consequently about the factors that influence the dynamics of the crack [1]. In this work, we present numerical findings that demonstrate that tensile cracks (mode I) can exceed the Rayleigh wave speed. This is achieved by considering geometric non-linearities into the material model. These non-linearities are typically present in most materials but have often been overlooked in the context of dynamic fracture propagation. Our results show that incorporating these non-linearities enables supershear crack speed. Additionally, we observe a geometric non-linear length scale inherent to elastic materials that affects the crack-tip opening displacement, cohesive zone behavior, and the energy flow around the crack tip. These findings imply that the elastic fields and energy distribution near the crack tip of geometrically non-linear materials significantly differ from those predicted by conventional linear elastic models in LEFM theory. This, in turn, offers a new perspective on dynamic crack propagation that questions existing theoretical models.

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Strain Rate-Dependent Constitutive Modelling of CFRP Laminates: Viscoelasticity, Viscoplasticity and Viscodamage

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ABSTRACT

A 3D constitutive model is developed to capture the strain rate-dependent behaviour of carbon fibre reinforced polymer (CFRP) laminates under different loading conditions. Building on a previous strain rate-independent framework [1,2], this model incorporates strain rate effects by combining several approaches. The viscoelastic response is represented by a generalised Maxwell model, while an overstress model [3] accounts for viscoplastic deformations. In addition, a novel viscodamage model is introduced to simulate both the initiation and evolution of damage at different strain rates. This viscodamage formulation extends a quasi-static damage model by using experimentally derived strength-strain rate relationships to adapt it to dynamic scenarios. To ensure numerical stability, the energy dissipation due to viscodamage is regularised based on the characteristic size of the finite element.

The predictive capability of the model is demonstrated by finite element simulations. It effectively captures the stiffer stress-strain response of CFRPs at high strain rates. In relaxation tests, the model shows how viscodamage initiates and develops without additional strain, as the material strength decreases faster than the stress level.

The validity of the model is further assessed by comparing the numerical results with experimental data from off-axis compression tests at various loading rates [4]. The comparisons show strong agreement in the viscoelastic, viscoplastic and viscodamage regions, confirming the ability of the model to reproduce the mechanical behaviour of CFRP laminates under dynamic loading conditions. Furthermore, the numerical predictions of quasi-static test results agree well the experimental data both the proposed and the original strain rate-independent model. Despite these promising results, further experimental work is required to improve the understanding of damage initiation and propagation under dynamic loading.

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Microscale and lattice-based modelling of brittle materials under dynamic loadings : application to porous ceramics

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ABSTRACT

The porous-cracked microstructure of plasma-sprayed ceramics coatings directly influences their macroscopic mechanical response. A 3D micromechanical model based on the discrete element method (DEM) is developed to reproduce their behavior. 3D observations are conducted with FIB-SEM nano-tomography and image analysis is used to extract and discretize the microstructure [1]. A modeling strategy is developed to incorporate both pores and cracks into the model while preserving the computation performance. The lattice nature of DEM [2] is used for the modeling of crack thicknesses that are smaller than the discrete element size. A method to compute the crack thickness from gray-level images is proposed. Virtual quasi-static tests are performed on a sample of yttria-stabilized-zirconia. The results are in accordance with the literature data, such as the anisotropy and the non-linear behavior related to fracture or high-pressure state. The model is helpful to precisely investigate the role of the microscopic components and micro-cracking on the macroscopic failure.

The effect of porosity on mechanical properties in intense dynamic regimes, including the propagation of mechanical waves, their attenuation and induced damage, as well as a detailed understanding of the mechanisms behind the observed behaviors, remains an area of investigation. Laser-driven shock wave experiments were simulated to study the compressive wave propagation into these kinds of porous brittle materials. 2D simulations using the present model are performed. The microstructure is reproduced using SEM observations. Both experimental and numerical results show that the crack thickness plays a significant role in the mitigation of shock wave intensity.

Finally, in order to study the influence of the microstructure of brittle materials on their dynamic and fracture behavior, the present model is used on a synthetic porous sample. A protocol for simulating uniaxial tensile tests is proposed, with the use of a heterogeneous initial velocity field that enables high strain rates to be achieved while ensuring balance of forces. The results in terms of maximum stress increase, cracking and stress field are analyzed in light of what is known in the literature.

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On the Interaction of Elastic Waves with Regularized Cracks in Gradient Damage Models

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ABSTRACT

The modeling of dynamic fracture is essential to understand failure mechanisms in structures subject to high strain rates, impact loading or seismic events. The phase-field fracture model [1,2] is a well-known approach to predict the fracture behavior of brittle materials. It is based on the regularized representation of a crack through a spatially varying damage variable (also termed the phase-field parameter) that locally degrades the elastic properties of the material. Although originally proposed in the quasi-static regime, extensions of the phase-field approach to the dynamic framework [3,4] are available and demonstrate potential to predict various realistic cases, including crack branching phenomena, mode-I crack propagation at velocities below or approaching the Rayleigh wave speed [5], and the emergence of crack-tip instabilities related to competing intrinsic length scales [6].

In the dynamic context, however, the spatial degradation of the elastic parameters at a crack introduces elastic wave reflections that result in spurious oscillations in the solution fields. In this contribution, we investigate the interaction of elastic waves with the regularized cracks by means of semi-analytical and numerical experiments and considering different phase-field formulations. First, we consider a simple one-dimensional bar containing a central fracture and we compare the amount of energy transmitted and reflected at the crack location. We then extend our study by considering common two-dimensional problems found in the literature and by analyzing the effects of the interaction between wave propagation and varying elastic parameters on crack nucleation and propagation. Alternative formulations are finally considered in order to assess their capabilities to overcome the mentioned drawbacks.

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Minisymposium EFE:

Enriched finite element formulations for fracture

Organized by B. Sluys and J. Alfaiate

Enhanced Beam Finite Elements with Enriched Kinematics for Objective Cracking Analysis of RC Beams

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ABSTRACT

This study presents advancements in the modeling of reinforced concrete (RC) frame elements using enhanced beam finite elements (FEs) with enriched kinematics to address objectivity issues in describing the onset and propagation of cracking. Conventional FE approaches that rely on classical displacement-based (DB) and force-based (FB) formulations suffer from mesh dependency and localization issues [1–3]. Hence, these approaches cannot capture complex cracking phenomena accurately [4,5]. To overcome these limitations, this research introduces an enhanced FB formulation that explicitly incorporates higher-order kinematics to include warping effects and better represents the localized cracking paths evolving in RC structural elements [6].

The proposed model addresses the limitations of the perfect bond assumption between concrete and reinforcement by including bond-slip effects [7] and adopts fracture energy-based regularization techniques [8]. By integrating refined numerical strategies such as higher-order interpolation functions for warping and improved numerical integration schemes [9], the enhanced FE formulation achieves objective results that realistically capture crack initiation and propagation.

Comparative analyses between classical and enhanced FEs illustrate the objectivity problems inherent in classical approaches and demonstrate the superior performance of the enhanced formulation. Validation through numerical test cases highlights the ability of the proposed modelling approach to converge effectively and provide a realistic description of the cracking behaviour [6].

The results emphasize the relevance of including enriched kinematics in beam FE formulations, thus offering a robust methodology for cracking analysis of RC structures. This work shows the practical implications of adopting enhanced FE formulations to improve the predictive capabilities of nonlinear FE models in structural analysis or RC frames and establishes a benchmark reference for future research in this domain.

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Crack Branching and Merging Simulations with the Shifted Fracture Method

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We propose a relatively simple and mesh-independent approach to model crack branching and merging using the Shifted Fracture Method (SFM), within the class of Shifted Boundary Methods. The proposed method achieves mesh independency by accurately accounting for the area of the fracture surface, in contrast to traditional element-deletion/node-release techniques. In the SFM, the *true* fracture is embedded into the computational grid, but the fracture interface conditions are modified (shifted) by means of Taylor expansions to the *surrogate* fracture composed of full edges/faces in two/three dimensions. This avoids numerical integration on cut elements, so that the data structures and geometrical treatment of cut elements are simple, while mesh-independent results and accurate fracture approximations are still maintained. We demonstrate the capabilities of the proposed approach in a number of prototypical numerical experiments.

MODELLING CORROSION IN REINFORCED CONCRETE USING A TOTAL ITERATIVE APPROACH

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Keywords: *Corrosion, Reinforced Concrete, Total Iterative Approach.*

Corrosion of steel in reinforced concrete structures is one of the main causes of structural deterioration, which leads to increased deformation, cracking and premature failure. In the present work, macro-mechanical modelling of corrosion is performed. A mixed-mode damage model is adopted [2], in which localised cracking is modelled by a discrete crack approach. Several factors are taken into account, namely: the degradation of the bond-slip relationship, the reduction of the sane cross section of the reinforcement bars, the rate of corrosion due to the environment, the compressive strength and the stress state in the neighbourhood of the concrete-steel interface, which can lead to an increase of the bond strength under compression, or to a decrease of the bond strength under tension. Special attention is given to the the passive evolution of corrosion, which aects the structure in time. In this case, degradation occurs under stabilised loading, with corresponding stiness decrease. The increase of corrosion leads to an increase of damage at the bond-slip level. A Total Iterative Approach (TIA) is adopted in the present work [1], in which the structure is reevaluated each time step, upon damage increase due to corrosion. Pullout tests are presented to evaluate the performance of the material model and bending tests are also performed to evaluate the inuence of corrosion at structural level.

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Minisymposium FFM:

Finite fracture mechanics: Models and applications

Organized by V. Mantič, A. Sapora and I. García

Crack Path in Compact Tension Cracked Specimens: Experiments vs. Phase Field model and Finite Fracture Mechanics

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ABSTRACT

Depending on the specimen geometrical features and crack initial length, the crack in Compact Tension specimen can propagate collinearly or branch, eventually following a curved path. Several approaches have been proposed in the literature to study this phenomenon under certain simplifying assumptions, with different complexity depending on the number of involved parameters, including T-stress [1] and Generalized Strain Energy Density (GSED) criteria [2].

The present work is devoted to the prediction of crack growth in brittle precracked Compact Tension geometries under Mode I loading using Phase Field (PF) model. The numerical approach combines a hybrid method that first employs a quasi-static analysis to capture the elastic phase of the tensile test, followed by a dynamic analysis to catch the nature of unstable fracture phenomena [3].

Accounting for the transition from stable to unstable propagation, a comprehensive analysis of the Energy Release Rate during the propagation phase is also conducted to verify that crack propagates in accordance with Griffith's energy criterion. Numerical outcomes are compared with experimental results reported in the literature [2]: PF analysis reveals to be able to predict the crack path deflection for the analysed geometries with sufficient accuracy.

Lastly, PF numerical results are compared with Finite Fracture Mechanics predictions [1] to assess the consistency and validity of the proposed model.

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Mechanical integrity of polymer film used in microelectronics: a identification of the thermoelastic properties and a coupled criterion analysis of the failure properties

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ABSTRACT

Polymer films are used in microelectronics at various stages of the stacking, in various applications. Their thickness is of some microns, and specific techniques are required to identify their thermoelastic properties. The latter are necessary to predict the mechanical integrity of heterogeneous multi-layers subjected to thermal cycles of various amplitudes during the processing and in-use.

We start by presenting a characterization method based on the curvature variation with temperature of a polymer film deposited on a silicon wafer [1]. An inverse problem is set from which the thermoelastic properties are derived, namely the in-plane modulus and coefficient of thermal expansion (cte). These are dependent on the magnitude of the Poisson's ratio. A 'realistic variation' of this quantity allows to derive the Young modulus and cte within an interval which is discussed together with the uncertainties related to the inverse problem formulated. The estimations are cross-compared with measurements from other techniques (colored ultrafast acoustics for the mechanical properties and temperature-dependent ellipsometry for the cte), with a good agreement.

With these estimations, we address the problem of assessing the mechanical integrity of a micron-scale structure made of a polymer pillar, of which height ranges from two to four microns, the width being several times larger. Along the polymer surface, a thin glass film is deposited, of which thickness ranges from 0.2 to 0.4 micron. The structure exhibits a large thermomechanical contrast, the hard glass coating being brittle. Depending on the thickness ratio between the polymer and the hard coat and the thickness of the latter, failure of the glass film is observed or prevented for a relative temperature variation of 300 K. The origin of this is discussed, and the failure properties of the encapsulating layer, namely its material's strength and critical energy release rate, derived by carrying out a Finite Fracture Mechanics analysis to the brittle layers following [2] and inspired by [3] within the context of thin brittle layers. This brittle coating is free is geometric singularity but a stress concentration arises from the elastic mismatch between the glass layer and the polymer pillar. Thanks to observation of safe versus brittle configurations, the brittle coating strength and critical energy release rate are identified. This allows the definition of the 'domain of mechanical integrity' by considering the polymer-to-hard coat thickness ratio and in particular the hard-coat thickness.

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Multi-site Damage Prediction using the Principle of Minimum Total Energy subjected to a Stress Condition (PMTE-SC) in Spring Interfaces

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ABSTRACT

A computational algorithm based on the Principle of Minimum Total Energy subjected to a Stress Condition (PMTE-SC) is used to study one of the main failure mechanisms in composites: debonding along fibre matrix interfaces under monotonic transverse loads.
The symmetric and non-symmetric character of the debond onset and growth is discussed in terms of the interface and bimaterial system parameters. The effect of deterministic and probabilistic generation of initial configurations of damage distribution along the matrix-fibre interfaces on the performance of the Alternating Minimisation Algorithm (AMA) applied to minimise the separably convex total energy functional is studied, focusing on the obtained optimum cracked configuration and the associated critical failure load. The bimaterial system considered includes: a glass fibre and an epoxy matrix; two glass fibres in proximity with the secondary fibre is oriented at 0, 45 and 90 degrees relative to reference fibre and the applied load. The current algorithm uses a two-dimensional (2D) plane strain formulation in the finite element code Abaqus, together with Python scripts that perform a time-stepping procedure that minimizes the total energy functional using the AMA. An efficient and adaptive load bisection algorithm is implemented that finds the failure load under a given user tolerance, avoiding the need for a constant load step scheme. The behaviour of the fibre–matrix interface is modelled by adapting the previously implemented Linear-Elastic Brittle Interface Model (LEBIM) programmed by means of a User Material Subroutine for Abaqus.
Finally, an analysis of the crack pattern generated by multiple fibre-matrix debonding is carried out, as it can result in a crack path (transverse crack in the 90° layer) or in an isolated fibre-matrix debonding.

Crack Velocity Profile Analysis During Crack Initiation

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ABSTRACT

The coupled criterion (CC) [1] enables studying crack initiation in various configurations [2]. The CC was originally established under a quasi-static framework, assuming "instantaneous" crack initiation at a given loading level and thus disregarding the actual way the crack forms during initiation. The CC formulation was since then refined in order to consider the kinetic energy variation during initiation by describing the initiation crack velocity profile [3,4]. It was shown that considering dynamic crack initiation, the initiation loading increases when the mean crack velocity increases as a larger crack velocity decreases the incremental energy release rate [3]. It was also shown that for a given mean crack velocity during initiation, the crack velocity profile has a first order influence on the initiation loading [3,4]. The determination of the crack velocity profile during initiation is thus crucial for accurately predicting the initiation loading in configurations where the mean crack velocity during initiation is not negligible.

This work aims at providing a method to determine the crack velocity profile during initiation. It is based on the simultaneous fulfilment of i) the CC and ii) dynamic propagation conditions. The proposed approach allows the optimal crack velocity profile during initiation to be determined numerically. Its implementation is illustrated on two examples, including crack propagation in an infinite medium and crack initiation in a specimen with a hole.

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Challenges for the FFMCC – Predicting fracture load for V-notched specimens under pure Mode III and for quasi-brittle materials

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ABSTRACT

The finite fracture mechanics coupled criterion (FFMCC) has demonstrated high accuracy in predicting fracture loads for brittle materials with V-notches. This has been validated through experiments conducted under mode I, mixed mode I & II, with both sharp and blunt V-notch tips.

However, extending the FFMCC to predict fracture loads for quasi-brittle materials (exhibiting small-scale yielding at the V-notch tip) or for V-notches subjected to pure mode III loading has proven challenging.

Here, we present experimental results from V-notched specimens made of quasi-brittle materials and ceramic cylinders with V-notches under torsional loading. The experimental fracture loads and torques are compared with FFMCC predictions, and the implications of the findings are discussed.

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COMPUTATIONAL IMPLEMENTATION OF THE COUPLED CRITERION OF THE FINITE FRACTURE MECHANICS

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ABSTRACT

The coupled criterion of finite fracture mechanics [1] has proven to be a criterion capable of predicting crack initiation in a wide range of problems of interest. Therefore, it is a good complement to Griffith's criterion, as it addresses one of its main limitations: the inability to predict crack initiation.

Due to its formulation, the coupled criterion can easily predict solutions using analytical or quasi-analytical methods in relateively simple problems [2]. However, its implementation in a purely numerical context is limited to advanced users within the finite fracture mechanics community, as there is no universal implementation. In this sense, several proposals can be found in the literature, see e.g. [3], and some projects are under development [4].

This work aims to address this limitation by proposing an implementation based on a very popular commercial code, allowing users to use it without advanced knowledge of finite fracture mechanics. To achieve this, the criterion is implemented using advanced tools already available in commercial codes, such as XFEM, and framed within the context of a multivariable optimization problem, where the geometry of the initiated crack is the optimization variable and the critical load at which the crack initiates is the objective function to minimize.

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Analysis of crack initiation in layered systems using a closed-form analytical approach

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ABSTRACT

Multilayer systems are used in various applications within mechanical engineering, electrical engineering or aerospace engineering, where they are exposed to thermal and mechanical loads. Within this work, a three-layer system is considered, which can serve as a model for several of these applications, for example for bonded joints with thick adhesive layers or for sandwich structures. It is common for such structural systems such as bonded joints or sandwich structures that the adherends or the outer layers are made of very stiff materials and the adhesive or inner layer is made of a more flexible material. A typical failure case in such layered structures is the development of interlaminar cracks leading to the delamination of individual layers. Because of the geometry and the dissimilar material properties of the layers, stress concentrations occur at the interface, which reach their maximum at the edges of the layer. These stress concentrations can lead to the formation of delamination cracks.

To predict the formation of interlaminar cracks, within the framework of finite fracture mechanics, a coupled failure criterion is used, which was postulated by Leguillon [1]. This criterion requires the determination of the stress distribution within the given structural situation and the incremental energy release rate for potential delamination cracks. For this kind of situation, a closed-form analytical approach is developed, which uses a higher order displacement approach to approximate these quantities very efficiently and accurately. To validate the model, the results are compared with finite element calculations.

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FINITE ELEMENT ALGORITHM FOR ANTIPLANE PROBLEMS WITH ONE OR MORE GURTIN-MURDOCH MATERIAL SURFACES

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ABSTRACT

Ultrathin and stiff layers, often encountered in microstructured systems and composite materials as coatings or embedded inhomogeneities, pose significant challenges in stress and displacement analysis. Recent advancements suggest these layers can be effectively modeled as material surfaces [1,2], following the theoretical framework developed by Gurtin and Murdoch [3,4] in the 1970s.

In a previous work [5], a finite element algorithm was developed to address antiplane elastic problems involving domains with boundaries coated by thin and stiff layers. These layers are treated as Gurtin-Murdoch material surfaces with vanishing thickness, which can be open or closed, and smooth or non-smooth. The governing equations are derived using variational principles, and triangular finite elements are employed to discretize the domains. Standard linear elements approximate displacements within the domain, while a novel blended singular element captures the singular elastic field behavior near the tips of open surfaces. Numerical examples demonstrate the accuracy and robustness of the proposed approach. This study has been further extended to analyze the interaction between two ultrathin and stiff platelets embedded in an isotropic matrix. Using the Gurtin-Murdoch surface model, the numerical analysis explores the influence of platelet distance and material properties on stress distribution. Key governing parameters are identified, and results provide insights into the mechanical response of such systems. Once the stress fields near the material surfaces are accurately modeled, various theories, such as the Coupled Criterion [6], can be employed to investigate crack initiation and propagation near the tips of ultrathin and stiff layers.

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Quantification of mechanical properties in cement lines using finite fracture mechanics

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ABSTRACT

The mechanical characterization of bone tissue presents significant challenges. Researchers often estimate the fracture toughness of cortical bone constituents at the microscale by combining experimental testing with numerical simulations. This work presents a first approach to the application of finite fracture mechanics for the estimation of fracture toughness and strength in cement lines. Different interface failure models based on the coupled criterion [1], considering shear stresses and mixed-mode loading, are evaluated in an inverse problem analysis in order to estimate the material properties of cement lines in conjunction with experimental data [2]. In addition, simulations with a cohesive zone model using the estimated properties via finite fracture mechanics showed strong agreement with experimental results, accurately predicting crack initiation within the cortical bone microstructure.

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Three-Dimensional Finite Fracture Mechanics Framework for Predicting Free Edge Delamination and Fatigue Life in Laminates

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ABSTRACT

This study introduces a comprehensive three-dimensional (3D) Finite Fracture Mechanics (FFM) framework to predict free edge delamination and fatigue life in laminated composite materials under various loading conditions, including mechanical, thermal, and cyclic loads. Delamination arises due to localized singular interlaminar stresses caused by the elastic mismatch between adjacent plies. The framework models delamination using a semi-elliptical crack geometry and couples material intrinsic properties, such as fracture toughness and strength, within the FFM criterion. Dimensional analysis, combined with Finite Element Method (FEM) simulations, is employed to derive generalized non-dimensional functions for stresses and energy release rates. These functions, validated against experimental data for a wide range of laminate configurations, allow the prediction of delamination without recalculating the boundary value problem for varying geometries and loading conditions.

For thermal loading, the FFM approach simplifies the prediction process by leveraging semi-analytical expressions derived from dimensional analysis. These expressions are independent of specific thermal loads and ply thicknesses, significantly reducing computational effort while maintaining accuracy. Validation against numerical models and experimental data demonstrates the framework's capability to predict delamination under thermal effects efficiently.

The framework is further extended to fatigue life estimation by incorporating interface properties as functions of the number of cycles. A quadratic relationship between the critical incremental energy release rate and the remote cyclic stress is assumed, enabling the development of a 3D FFM fatigue criterion. This criterion is solved through constrained nonlinear optimization, providing predictions of finite fatigue life for different laminate configurations. Results highlight the influence of ply orientation angles, showing that lower angles enhance fatigue performance. The model predictions exhibit close agreement with experimental findings from the literature. The unified 3D FFM framework provides a robust and efficient tool for analyzing delamination and fatigue behavior in laminated composites, offering valuable insights for the design and optimization of advanced composite structures.

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Optimal geometry in two-steps lap joints: Cohesive Zone Model vs. Finite Fracture Mechanics approach

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ABSTRACT

Considering load transfer between different joining elements, adhesively-bonded joints are commonly preferred over other traditional joining methods, i.e., mechanical joints with fasteners, because of numerous advantages. The latter include their light weigth, the possibility to join structural components without strength reduction due to fastener holes, uniform stress distribution, impermeability, and so on. In this context, different configurations of adhesively-bonded joints, such as single-lap joints, butt joints, scarf joints, and stepped-lap joints, are possible [1]. The stepped-lap configuration gained significant attention due to their inherent capability of reducing stess concentration (peeling stresses) at the joint ends, thus enhancing the bond strength. Several scholars focused on the influence of the step length and of the step number on the load capacity [2, 3], but limited studies discussed the effect of the step height.

In this work, the load capacity of two-steps lap joints made of similar adherends is analyzed, by assuming a linear elastic behavior of the adherend and a rigid-linear softening cohesive law at the interface. The focus is on the *optimal shape* of the two-step configuration, i.e., the step height providing the maximum transferable load, together with the related *effective bond length*, i.e., the bond length required to transfer that load. The analytical solution highlights the following trends: (i) a relationship between the maximum transferable load and the bond length is found, whose trend is the same regardless to the joint shape (defined by a dimensionless parameter α); (ii) the bond strength is maximized when the optimal configuration, described by $\alpha = 0.25$ ("one fourth rule"), is adopted. In this sense, the latter result is consistent to the numerical findings recently reported in [4]. Finally, the same structural problem is faced by Finite Fracture Mechanics [5], yielding the same joint optimal shape but slightly different bond strengths.

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Fracture and damage of composites and laminates

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Higher-order finite beam models for progressive damage analysis of composite structures based on 3D Tsai-Wu orthotropic damage model

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ABSTRACT

This study investigates the progressive damage analysis of orthotropic composite structures under quasi-static loading using a higher-order beam model coupled with an orthotropic damage model based on the three-dimensional (3D) Tsai-Wu failure criteria. The higher-order beam model is derived within the framework of the Carrera Unified Formulation (CUF), which provides the 3D displacement field of beam model through cross-sectional expansion. Therefore, quasi-3D stress state can be obtained with improved computational costs compared to fully 3D models. Within the CUF framework, the Node-Dependent Kinematics (NDK) approach can be employed to further reduce computational costs without sacrificing too much accuracy. The orthotropic damage model used in this work independently accounts for fiber, matrix, and out-of-plane damage once the Tsai-Wu failure criterion is satisfied. To mitigate mesh dependency issues commonly associated with continuum damage models, the fracture energy regularization technique is incorporated into the damage progression. Comparative analyses of numerical and experimental results demonstrate that the proposed models accurately capture the load-displacement behavior and damage patterns of composite structures, providing an efficient and reliable tool for simulating progressive damage analysis.

A two-scale approach unravelling process-induced delaminations in polymer-coated metal sheets causing air entrapment

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ABSTRACT

Packaging steels are typically coated with PET-polymers for preserving content quality, preventing corrosion, and enabling printability on the surface. The industrial lamination process handles large volumes at high speeds, whereby it has been reported that air bubbles get entrapped between the polymer coating and the steel substrate, significantly impacting the final product's quality and lifetime. The root cause of this problem is assumed to be related to insufficient bonding or contact, which entails delaminated pockets with entrapped air at the interface.

The physics governing these delaminated areas (revealing a lack of bonding or contact) are poorly understood, and establishing the relationship with the applied process parameters is essential to prevent their occurrence. This contribution unravels this delamination and air entrapment problem using a two-scale modelling strategy, complemented by experiments. The coarse-scale model establishes the connection between the processing parameters (line speed, roll pressure, temperature, etc.) and the actual loading conditions in the lamination nip where the polymer film is supposed to bond. The fine-scale model delves into the roughness asperities of the steel sheet, explicitly studying the plastic flow of the film at high temperature and strain rates into the roughness valleys. The Eindhoven Glassy Polymer [1] is employed to model the behavior of PET under extreme rate/temperature conditions, where thermo-mechanical parameters are taken from literature or identified from experiments. The micro-scale model allows to study the non-contact of insufficiently bonded regions.

The results from the two-scale finite element model reveal that delaminated pockets (with air bubble formation) are most prominently present when the temperature of the substrate steel is too low or lamination speed is too high. The model unravels the microscale parameters that govern inadequate bonding at the metal-polymer interface. Moreover, it also establishes a quantitative relation between macro-scale process parameters on the one hand and the micro-deformation of PET at the micro-scale inducing incomplete filling or bonding. The model presented is a nice illustration how fine scale simulations may be exploited at engineering scales for materials processing.

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Fracture Energy-Based Damage Simulation of Pultruded GFRP Materials at Different Temperatures

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ABSTRACT

The numerical simulation of fracture and damage of composite materials has been a challenging issue, particularly for structural-grade pultruded fiber reinforced polymer (FRP) materials, which are characterized by significant thicknesses (>5 mm) and complex fiber layup configurations. Previous studies [1-2] successfully implemented Hashin criteria alongside the fracture energy-based damage evolution tool of ABAQUS [3] (i.e., linear cohesive law) to simulate the transverse fracture behaviour of these materials. These simulations, validated by test data, were performed using shell finite element (FE) models, where the material properties were assumed to be orthotropic and homogeneous through the thickness, which are reasonable simplifications for in-plane analyses. However, there has been no research on the fracture behaviour of FRP composites at elevated temperatures. Since pultruded FRPs are sensitive to high temperatures that may occur in outdoor service conditions, accurate damage simulation of their failure under such conditions is essential. In this context, this paper presents an experimental and numerical investigation on the transverse fracture behaviour of pultruded glass-FRP (GFRP) materials at different temperatures (20/40/60/80℃). Wide compact tension (WCT) fracture experiments were simulated with FE models, and the load *vs*. displacement curves were compared (including ultimate loads and softening slopes). Alongside the linear cohesive law, an exponential cohesive law was also implemented through user defined material subroutines (UMAT) in ABAQUS. The results demonstrated that the experimentally-based fracture energies, applied within the framework of both cohesive laws, provided good agreement between numerical and experimental results. The best correlation was achieved using the linear cohesive law, with the material strength obtained from mechanical characterization tests.

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Certification supported by simulation of bolted structures

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ABSTRACT

Despite the ability of new manufacturing processes to produce very large composite structures, single stage processed parts remain highly challenging. In aeronautics, composite parts are preferably assembled with fasteners, mainly for repair and certification purposes. The work presented here aims at demonstrating that simulation can support the certification of bolted structures and help to reduce the amount of tests required. The building block approach was applied to bolted L-shaped components [1] with two types of unit test considered: an unfolding test of an L-shape specimen and a pull-trough test of a bolted plate.

Tests and simulations were performed on carbon/epoxy laminates with multiple configurations in order to evaluate the capability of the modelling strategy to predict the mechanical response of the composite parts in the pull-through and the unfolding tests. Tests instrumentation included Digital Image Correlation (DIC) to capture displacement fields and damage. Models of pull-through and unfolding tests were developed and used to simulate the various configurations that were tested. A constitutive law based on a combined 3D plastic-damage model was used to describe the response of the composite materials [2].

In order to improve the confidence in the modelling strategy, the models will be implemented into a platform called VIMS (*Virtual testing integration platform for decision making support*) to enforce a rigorous VVUQ process [3]. The process starts with a robust calibration based on previous sensibility analyses identifying relevant calibration tests and ensuring the influence of the model parameters are well captured. Verification and validation tools are implemented to support the verification of the model implementation and evaluate the model's validity domain along with an estimated error of the numerical predictions. Comparisons with experimental data, and in particular DIC, will provide information on damage mechanisms and failure modes to support a thorough validation. The final objective is to compute design values for the bolted L-angle specimens using simulations.

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Data-Driven Fracture Characterization of Composites: A Non-Black-Box Approach

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ABSTRACT

This study presents a transparent, data-driven approach for the certification and characterization of composite materials, utilizing the Gauss-Newton (GN) algorithm to achieve high accuracy and computational efficiency. The proposed method focuses on predicting the mechanical properties and the coupon strength of the carbon fiber-reinforced polymers (CFRPs). Unlike traditional black-box models (e.g., machine learning models such as XGBoost, Random Forest, Artificial Neural Networks, and Gaussian Processes), the proposed approach can establish a clear mathematical pathway from input to output while requiring significantly fewer training parameters.

The transparent mathematical framework proves valuable in establishing relationships among mechanical properties of materials and reduces characterization costs by replacing experimental approaches with mathematical representations. Additionally, the GN algorithm's simplicity enables the identification of relationships between related parameters with fewer training samples. The potential applications of the GN algorithm are demonstrated through invariant-based calculations of the mechanical properties of composites: Young's modulus [1], strength, and fracture toughness [2].

Another key application of the GN model is the prediction of coupon strength. In this study, we analyse the open-hole tensile (OHT) strength across various composite configurations, including different CFRPs, layup sequences, diameter sizes, and width-to-diameter ratios, to provide a comprehensive understanding of a coupon certification process with multiple variables. The methodology involves generating training data through a combination of finite element method (FEM) simulations and experimental results. The testing results show that the GN model effectively predicts OHT strength and demonstrates robust performance across diverse test cases.

The findings underscore the efficiency and interpretability of the GN-based approach, offering a robust and transparent alternative for reliable certification and characterization methods for composite materials.

ACKNOWLEDGEMENTS

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Investigation of Delamination and Matrix Cracking Behavior in Z-Shape Laminate using Phase Field Model – CFRAC 2025

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ABSTRACT

The study investigates the delamination and matrix cracking behavior of Z-shaped thermoset composites through experimental and numerical methods. The specimen is fixed at one end, while the other end is subjected to quasi-static loading at a rate of 5 mm/min. This loading induces mixed-mode failures, including bending-opening and tension at the corners (see Figure 1A). In the context of the numerical model, a damage-driven Phase Field (PF) approach is implemented [1]. Structural tensors are employed to adapt the stress-based failure criteria, accounting for inherent transverse isotropy. This modification is integrated into the cracked PF evolution equation, resulting in a robust mixed-mode 3D framework. Furthermore, regarding the optimal characteristic functions of the PF model, a PF-regularized cohesive zone model with a linear softening law is applied to brittle fracture. This approach employs a strength-based crack initiation criterion to compute delamination and matrix cracking paths in a unified manner. The approach ensures that the PF model parameter, represented as a length scale, affects only the smeared crack width with minimal influence on the overall mechanical response. Additionally, discontinuities such as voids are examined after manufacturing using an optical microscope, along with process-induced distortions caused by locked-in residual stress fields, prior to conducting the structural analysis. In the numerical model, the effects of manufacturing defects, specifically voids and residual stresses generated during part processing—are incorporated using a heat transfer analogy. This approach ensures that all post-manufacturing information is retained [2]. The cure-induced residual stress field is numerically simulated using a viscoelastic constitutive model and validated by comparing process-induced distortions, represented as spring-in angles. Numerical results, both with and without the presence of manufacturing defects, are compared with experimental data obtained in the study. The results (see Figure 1B and 1C) are thoroughly analyzed to explore various delamination initiation, migration, and matrix cracking behaviors.

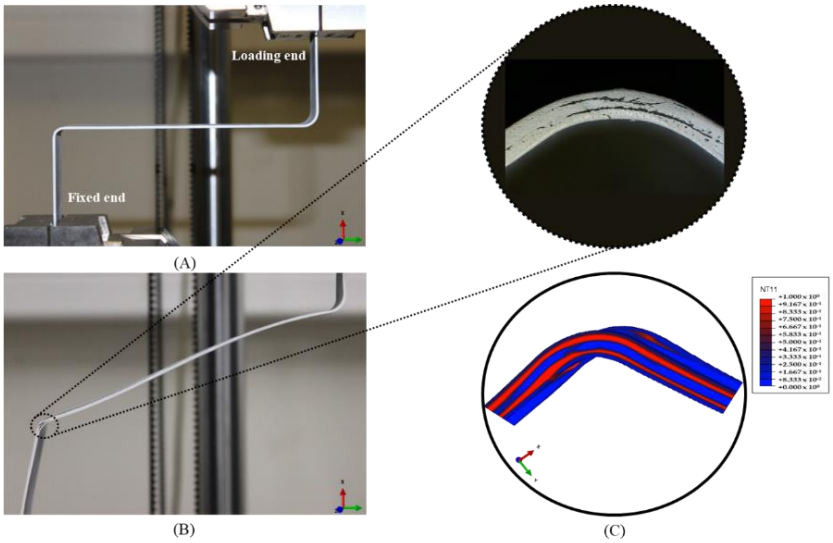

Figure 1. (A) Illustration of the mixed-mode failure test in the Z-shaped part, accompanied by a comparison of delamination and matrix cracking between (B) the experiment and (C) the numerical PF model.

Keywords: Phase field, damage, fracture, defects

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Lifetime Simulations of Hygro-Thermo-Mechanically Loaded Adhesive Bonds

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ABSTRACT

To reliably ensure the proper function and safety of adhesive bonds subjected to cyclic loading, temperature, and humidity, specialized computational models are required. In this symposium, we aim to present our simulation method, which enables the prediction of the lifetime of hygro-thermo-mechanically (HTM) loaded adhesive joints.

We hereby want to focus on the following aspects:

- **Solution of coupled multi-field problems:** We propose an approach for addressing coupled three-field problems involving mechanical, thermal, and diffusion processes, while improving numerical efficiency.
- **Formulation of a constitutive model for adhesives:** A viscoelastic material model, which incorporates the effects of temperature and water concentration through the time-temperature-concentration superposition principle, is coupled with a local damage formulation to model the degradation of adhesives. The damage evolution equation includes contributions from creep damage [1], fatigue damage [2] and hygroscopic damage [3].
- **Parameter identification:** Parameter identification methods based on experimental data provided by the Laboratory for Material and Joining Technology (LWF) at Paderborn University are presented, aimed at calibrating the model to real adhesive materials.
- **Outlook:** An outlook on remaining tasks in the project will be provided.

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Finite Element Modeling of Tapered Composite Laminates for Selective Interlaminar Reinforcement

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ABSTRACT

Composite laminate structures are often designed with tapered geometries to optimize weight distribution by terminating specific plies, referred to as ply drop-offs, in regions experiencing lower applied loads [1,2]. However, these regions are prone to stress concentrations that can result in interlaminar delamination, leading to premature failure [1,2]. To address this, aligned carbon nanotubes have been explored for selective structural reinforcement to suppress delamination onset at these critical interfaces, enabling more optimized designs with reduced weight. In this study, finite element modeling was utilized to develop tailored designs for a tapered composite laminate, incorporating selective reinforcement strategies. Tapered composite laminates were modeled and experimentally validated to assess static mechanical behavior. A parametric study was conducted to investigate the effects of ply stacking sequences, laminate geometries, and test configurations on stress distributions. The finite element models were able to predict the linear elastic behavior of the tapered laminate but were not used to predict progressive failure. The findings underscore the potential of selective reinforcement with aligned carbon nanotubes in mitigating delamination at ply drops, paving the way for lighter and more durable composite structures in aerospace applications.

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Revisiting Multi-Phase field model for FRCs using PUCK failure theory

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ABSTRACT

A multi-phase field damage model capable of handling both fiber and inter-fiber (matrix-dominated) fracture separately in Fiber Reinforced Composites (FRCs) is proposed in this work. The work utilizes the PUCK failure theory for the crack initiation based on the local stress state, whereas the phase-field method propagates the crack. The directional nature of the fracture energy stemming from the various fiber orientations is considered for realistic crack propagation. The shortcomings of the [1] are addressed in this work to enhance the prediction capabilities, implementation, and computational efficiency of the phase field model. Specifically, this work proposes a multi-phase field method relying on the PUCK failure criteria for triggering the fracture in fiber and the inter-fiber regions, using two independent phase-field damage variables in a thermodynamically consistent framework.

Furthermore, the formulation encompasses two different characteristic length scales and the structural tensor to enhance the accuracy of qualitative and quantitative prediction. Additionally, the present model accommodates various failure modes, orientations of the plies, and crack tip geometries. A total of seven benchmark examples will be used to demonstrate the model's predictive capability. Each example compares the present model to the experimental results using qualitative and quantitative analysis. As an example, Fig 1 presents the qualitative comparison between experiments conducted in [2] and the proposed work in the Centred Notched Tension (CNT) specimen. The extreme cases such involving fiber orientations of $\theta = 90^0$ with respect to loading direction are studied in detail to illustrate the interaction between the fiber and the inter-fiber failure, effectively capturing crack splitting shown in Fig 1e). Unnotched tension specimens are examined to evaluate the effects of artificial defects/voids on crack propagation in the FRCs in various ply orientations.

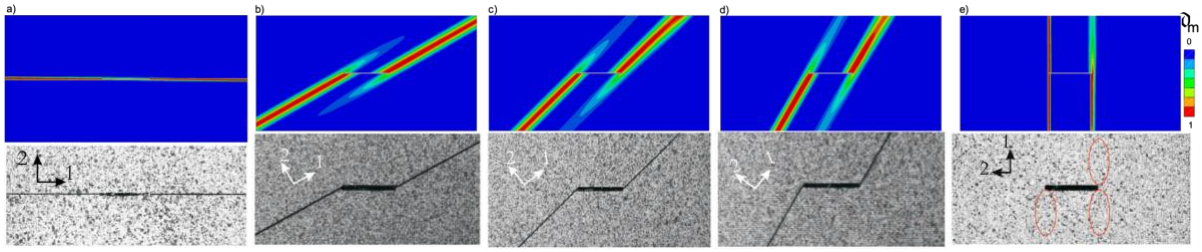

Fig 1: Comparison between the experimental observations from [2] and the proposed model for the fiber orientations of a) 0^0, b) 30^0, c) 45^0, d) 60^0, and e) 90^0. The experimental results are reproduced from [2] with permission from Elsevier.

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Geometry-controlled interlaminar resistance

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ABSTRACT

Composite materials have become integral to various industries due to their mechanical properties and adaptability to advanced manufacturing technologies. However, delamination remains a critical challenge, affecting the service life of composite structures by reducing stiffness and strength. Traditional approaches to mitigate delamination focus on enhancing interfacial properties through material modifications or surface treatments [1]. Recent studies suggest that altering the interfacial geometry offers a promising avenue for controlling delamination progression [2].

This work presents an analytical model that comprehensively describes the growth of planar cracks at width-varying interfaces within laminated materials. By examining width-tapered double cantilever beam (WTDCB) specimens, we define two key geometric parameters: the effective width rate and the crack growth plane shape factor. These parameters lead to a compact formula predicting the load response for arbitrary shapes, effectively bounding all planar delamination geometries through a family of similar power-laws.

Two analytical models are developed: an explicit model expressed using hypergeometric functions and an approximate model based on simplifying assumptions. The models describe the load-displacement response after crack propagation, providing insights into the relationship between force-law curves and sample geometry. Validation is achieved through numerical studies employing 3D cohesive zone models and experiments with carbon fiber laminates, demonstrating good agreement between models and experimental outcomes.

Our findings indicate that controlling the geometry of the crack growth plane can establish conditions for stable crack propagation, regardless of applied boundary conditions. An initial width approaching zero at the loading point prevents force reduction during displacement, while a larger initial width increases peak load but may result in force diminishment as displacement increases. Enhancing both the effective width rate and a shape factor different from unity improves force response during crack propagation.

Obtained results advances the understanding of fracture mechanics in composite materials and supports the design of fracture metamaterials—materials that increase their load-carrying capacity during crack propagation due to their geometry. The analytical models developed are valuable for designing and optimizing composites and composite patches with unique shapes and enhanced crack resistance. Controlling the crack growth plane shape and dimensions to improve load-carrying capacity and ensure fail-safe objectives may be more feasible than incorporating new materials or technologies to increase fracture toughness.

Finally, we have generalized the expression for the load response, demonstrating that geometry transforms the usual monomial relation between forces and displacements into a polynomial of order directly linked with the delamination shape.

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On the Impact of Initial Micro-Defects on the Transverse Failure of Unidirectional Composites using a Phase-Field Model for Brittle Fracture

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ABSTRACT

In the past decade, the continuous development of novel composite manufacturing technologies and processes played a pivotal role on the increasing employment of advanced structural composites. While this has demanded the establishment of adequate quality control procedures and nondestructive inspection protocols, there has also been a growing research interest on the properties and performance of composites in the presence of manufacturing defects.

Given the inherently multi-scale nature of composite materials, manufacturing defects may be found across various spatial scales, ranging from the laminate level to the fibre-matrix interaction domain. This contribution focuses on the effect of defects on the transverse failure of unidirectional composites at the microscopic scale. These defects are modelled as initial micro-cracks, with a predefined length and placed at random locations, to mimic the spatial distribution of flaws in the microstructure of a real composite material.

A variational phase-field model for brittle fracture is herein adopted to model the failure of unidirectional composite Representative Volume Elements (RVEs). Preliminary studies are conducted to estimate the properties of the pristine microstructures, where the effect of the RVE size is assessed. Subsequently, the study examines the effect of micro-defects by defining various types of initially damaged RVEs and generating multiple realizations for each type. The location and concentration of micro-cracks are seen to play the primary role on the reduction of the strength, strain at failure and toughness of the composite RVEs. In addition, the length and direction of the micro-cracks may also have a discernible impact in certain scenarios. Different tendencies are observed for different RVE sizes, with respect to the importance of the number and length of the micro-defects, and it is seen that these flaws can produce significant changes in the resulting crack path.

Damage modelling of fibre-reinforced polymer composites using a smeared crack approach – CFRAC 2025

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ABSTRACT

In this work, a novel formulation of the 3D smeared crack model for damage propagation under longitudinal and transverse failure modes is presented using a continuum damage approach. This formulation is developed to facilitate the implementation in an implicit solver, increasing solution robustness and computational efficiency in quasi-static and long-duration analyses. The constitutive model includes the material elastic plastic behaviour in the transverse direction, and failure initiation incorporates a stress-invariant approach for transverse failure and kinking failure, seamlessly integrated with the posterior damage evolution. The performance of the model is evaluated using monotonic and non-monotonic damage evolution, verified with single-element tests to demonstrate the consistency of the proposed formulation regarding failure load and energy dissipation. Additional benchmark examples, including off-axis and open-hole tests, are performed to validate the proposed modelling approach with experimental results. The results show good agreement with experiments for the predicted plastic response, failure loads, and notch size effect.

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Investigation on Mechanical Behaviours of Biaxially Woven GFRP laminate in Hygrothermal environments

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ABSTRACT

To investigate the mechanical behaviors of biaxially woven glass fiber reinforced plastic (GFRP) laminates under hygrothermal conditions, compression tests with and without holes, as well as in-plane shear tests, were performed under conditions (temperature: 23°C ± 2°C, humidity: 50% ± 5%) and (temperature: 70±2°C, humidity: 85±5%). Load-displacement curves, failure loads and failure modes were obtained. A progressive failure analysis model considering hygrothermal effects was proposed to predict the failure modes of specimens in hygrothermal environments. The three-dimension (3D) Hashin failure criterion was used for failure prediction. A hygrothermal strain constitutive equation was introduced, and a VUMAT subroutine was developed and embedded into the ABAQUS solver to establish an explicit finite element simulation model. This model accurately reproduces the test load-displacement curves from the initial loading point to the failure point, in good agreement with experimental data. Additionally, the model effectively identifies the damage onset and compares the damage propagation of specimens under these two environments, thereby offering guidance for engineering applications.

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Numerical modeling of 3D crack propagation in orthotropic composites using a massively-parallel, adaptive phase-field framework

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ABSTRACT

Prediction of cracks in orthotropic composites is important in various engineering applications such as aerospace, defense, and automotive. Phase-field fracture models have demonstrated remarkable effectiveness in simulating various real-life failure mechanisms in composites (intralaminar, interlaminar, and translaminar failure). However, most available phase-field fracture models remain two-dimensional primarily due to their high computational cost. We address this limitation and develop a massively-parallel and adaptively refined phase-field fracture model for orthotropic composites by extending the work of Jain et al. [1] to 3D. The framework is developed in the deal.II library [2] and capitalizes on two key features, parallel computing and adaptive mesh refinement, mitigating the computational demands associated with phase-field models in 3D. The model is validated against established benchmarks in the literature. Subsequently, we conducted a series of numerical experiments, demonstrating the framework's capability to solve complex 3D fracture problems. Here, we provide one such example demonstrating the fracture of an orthotropic composite laminate subjected to an Open-hole-tension (OHT) test. The laminate is composed of two laminae, one stacked over the other. The lower lamina has fibers oriented at $\theta = -\pi/4$, with respect to the x −axis while the fibers in the top lamina are oriented at $\theta = \pi/2$. The problem setup is shown in Figure 1. Figure 2 shows the damage contours from two different views. As expected, intralaminar failure occurs along the direction of the fibers in each layer.

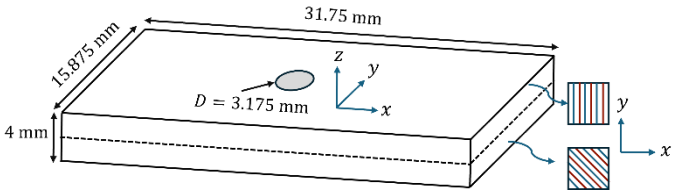

Figure 1: Schematic of the problem setup for the Open-hole tension (OHT) of a composite laminate.

Material parameter sensitivity analysis for interlaminar damage of laminated composite structures

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ABSTRACT

Understanding the relative importance of model parameters is a critical task in various fields, such as design optimization and uncertainty quantification [1]. Two distinct approaches can be employed to generate sensitivity information. The first involves sampling-based methods, often relying on machine learning techniques. These methods treat the model as a "black box," allowing the use of commercial codes without any further modification. The second approach involves generating local sensitivity information by linearizing the model response during its solution process [2], within the framework of the Direct Differentiation Method (DDM). Provided that an implicit solver is used, DDM can be applied to any analysis, static or dynamic [3], with only minimal extensions to the standard code to account for parameter linearization.

In this study, the damage behavior of laminated composite structures undergoing interlaminar damage is examined using DDM to assess the influence of material properties employed in cohesive models. Two different models are analyzed and compared: one featuring a commonly used linear softening approach [4] and another utilizing an exponential softening approach [5]. Simulations of structural details are presented, where damage is modeled exclusively at the interfaces to isolate cohesive damage effects.

To address the challenge of modeling larger structures and considering the highly localized nature of damage, a reduced basis approach is proposed for approximating the sensitivity response. A selection of basis vectors is constructed using pre-computed information during the iterative solution process, and the accuracy of this approach is validated against the full-system solution using the earlier examples.

Finally, more realistic aeronautical applications are presented. Simulations of three single-stringer compression specimens, including both pristine and pre-damaged configurations, are conducted using data from [6] and [7]. These simulations yield first-order variations of the response with respect to selected material properties (elastic, intralaminar, and interlaminar), enabling a first-order accurate estimate of response variability under uncertain material properties. At the peak load, because of the high gradients, where the linearization would not allow to estimate the variability of the response for larger variations of the material properties, the model is restarted from the linearized results and additional shorter analyses around the singular point are carried out. From these results, the variability of the maximum load is computed. Comparisons with reference solutions obtained via Polynomial Chaos Expansion (PCE) analysis show good agreement, with the proposed approach offering significantly reduced computational cost.

In summary, this work addresses three aspects: the application of DDM to interlaminar damage modeling of laminated composites, the development of a reduced basis method in the context of DDM, and the application of these methods to larger composite structures for first-order response variability estimation under uncertain material properties.

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Impact Response and Compression-After-Impact Behavior of Preloaded Composite Laminates: A Finite Element Analysis

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ABSTRACT

This investigation examines the low-velocity impact response (LVI) and compression-after-impact (CAI) performance of composite laminates subjected to preload conditions. A three-dimensional finite element model was developed and validated through experimental data under non-preload impact configurations. The validated numerical framework was subsequently extended to characterize the influence of tensile and compressive preloads on damage evolution, energy dissipation mechanisms, and failure modes in composite laminates under LVI. The analysis demonstrates that preload conditions significantly affect the CAI strength, with the degradation magnitude correlating to preload levels. Both tensile and compressive preloading promoted damage propagation and diminished CAI resistance. These computational predictions establish a theoretical foundation for characterizing laminate response under combined loading conditions, facilitating the development of optimal composite structural configurations.

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Fatigue Life of Tow Steered Composite Pressure Vessels

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ABSTRACT

Recently, there has been rapidly growing interest in hydrogen as an energy source in Europe and worldwide. One of the challenges in using hydrogen as an energy source in applications related to the transportation system is the need for efficient, lightweight pressure vessels with improved packing efficiency, which enables storing more media in the same amount of space and consequently enables travelling for longer distances without the need for frequent fuelling.

Stiffness tailoring can be used to provide a lightweight composite pressure vessel. Daghighi et al. [1] developed a design method based on stiffness tailoring by varying the fibre tow trajectory throughout the structure that can redistribute the stress gradient uniformly through the thickness, increasing the overall load-carrying capacity and significantly reducing weight. These advantages make their designed pressure vessels potential candidates for the next generation of pressure vessels.

Failure is an important factor in designing pressure vessels that should be predicted accurately in order to ensure a safe design. In this research, we investigate the failure performance of the proposed design for a family of pressure vessels and use a direct cyclic analysis procedure to obtain results that can be used for fatigue life calculation of tow-steered composite pressure vessels.

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A micromechanical framework for creep and fatigue modeling of composites combining viscoplasticity, cohesive damage and time homogenization

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ABSTRACT

Time-dependent failure of fiber-reinforced composite materials comprises a complex combination of phenomena which are not yet fully understood. An improved understanding of how composites fail under creep or fatigue loading is crucial in achieving lighter composite structure designs not heavily reliant on conservative safety factors. This is however a daunting endeavor: experimental investigations of creep and fatigue in composites are arduous and expensive, while an all-encompasing numerical modeling framework taking into account the wide range of complex failure mechanisms involved is essentially non-existent. Indeed, an accurate model should allow for both plasticity-controlled failure (frequency independent in time but not in number of cycles) and crack growth-dominated failure (frequency independent in number of cycles but not in time) to arise, as well as accurately modeling the transition between the two regimes and the influence of different load ratios.

In this work we present a micromechanical modeling framework that unifies fatigue and creep modeling with combined viscoplasticity and cohesive crack growth [1]. We consider unidirectional composites under off-axis loading, taking into account the effect of large strains and the influence of the reorientation of the fiber direction it entails. Special boundary conditions are used to enforce a uniaxial stress state on a rotating RVE in large deformations. A novel time homogenization algorithm is proposed that splits the equilibrium problem into micro- and macrochronological steps in order to improve the computational efficiency of micromechanical simulations involving a large number of time increments. To handle crack initiation and propagation, crack segments are inserted on the fly based on a novel initiation criterion and a cohesive zone model is employed allowing damage to evolve both quasi-statically and in fatigue.

We use the new framework to simulate the response of unidirectional carbon-PEEK samples and compare results from micromechanical simulations to creep and fatigue tests on coupons under off-axis loading. Fibers are modeled with a transversely isotropic hyperelastic model and the resin with the Eindhoven Glassy Polymer (EGP) model. We show that our models can correctly predict the transition between plasticity-controlled and crack growth-controlled failure and the associated frequency dependencies with remarkable accuracy. The model can also accurately predict material response under creep loading, although challenges remain in correctly predicting how the load ratio R affects failure.

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Uncertainty Quantification of Open-Hole coupons through a global-local approach with PC-Kriging surrogate modelling

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ABSTRACT

The response of composite structures is subject to uncertainty resulting from variability in material properties and the manufacturing process. High fidelity finite element simulations are capable of accurately predicting the behaviour of composite structures, but their high computational cost makes them prohibitive to generate sufficient data to characterize uncertainty, hence surrogate models become appealing. Adequate uncertainty quantification (UQ) allows for a greater understanding of the structural response due to variabilities, as well as an assessment of the computational models used for structural simulation [1]. UQ has the potential to change the current paradigm of the certification process, which relies on deterministic simulations with safety factors and extensive experimental campaigns, by reducing the experimental testing required and increasing the role of simulation in certification. In this work uncertainty quantification of Open-Hole (OH) coupons with aleatory variables is performed using surrogate models built on global-local simulations. The global simulations are carried out at the laminate level calculating the displacement field of the full coupon. Then local simulations are executed in a smaller region around the hole at the ply level with continuum damage mechanics transferring the displacements from the global simulations. Polynomial-Chaos-Based Kriging (PC-Kriging) [2] surrogate models are built from these simulations as a computationally fast alternative to evaluate the system response and allow for sampling over a large number of input parameters combinations. These surrogate models are used in this work to perform uncertainty quantification on the failure strength and other relevant properties of OH coupons. Sensitivity analysis is performed to quantify the influence of the input parameters on the behaviour of the coupons.

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Integrating Laminate-Level Bolted Joint Failure Envelope Data into Low-Fidelity Finite Element Models for Composite Joint Stiffness and Failure Prediction

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ABSTRACT

Current industry practice to connect composite structural panels still relies on the extensive use of bolted joints. However, because of their anisotropic nature, composite bolted connections represent a significant design challenge and have thus been the subject of ongoing research. While particular focus has been given to the in-plane and out-of-plane performance of mechanically fastened joints, real-life applications (e.g. L-junctions and single-lap joints of thin laminates) involve a combination of both loading scenarios that must be evaluated simultaneously [1,2].

A numerical approach to characterize the three-dimensional failure envelope of a directional carbon-fiber-reinforced composite joint is proposed for the first time. Eighteen high-fidelity tridimensional damage simulations that replicate the pure bearing, pure pull-through, and combined loading tests (developed in Ref. [3]) for several loading axes (longitudinal, transversal and off-axis) are run to obtain the first load drop of the joint. A failure envelope is then derived through the ellipsoidal fitting of the simulation results.

The proposed failure envelope is subsequently applied in the estimation of the failure condition in bolted single-lap joints suitable for large-scale structural models. Five multi-bolt single-lap shear joints are simulated using two distinct approaches: a non-linear high-fidelity method with three-dimensional elements considering ply and inter-ply damage, and a linear-elastic low-fidelity method utilizing shell and connector elements.

Results indicate that the methodology developed to numerically determine the bolt failure envelope, combined with the use of connector elements as fastener representatives, is appropriate to accurately simulate the joint stiffness and load ratios in the first failed bolt, and predict first-drop laminate-level failure in composite bolted connections while providing a substantial reduction in computation expenses, establishing their potential for future use in large-scale models.

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Multi-scale analysis of damage and fracture

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Prediction of mechanical properties using multi-scale approach for plain woven SiC/SiC composites

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ABSTRACT

Ceramic matrix composites are ideal materials for high-temperature components of aero-engines due to their excellent high-temperature mechanical properties and other advantages. Therefore, it is of great significance for the research and application of SiC/SiC composites to understand the strength and damage evolution mechanism under load. In this paper, based on the multi-scale characteristics and the periodicity of microstructure of plain woven SiC/SiC composites, the unit cell models of microscale (fiber-scale) and mesoscale (yarn-scale) are established. The mechanical properties parameters of the microscale model were calculated by Abaqus software, which were then introduced into the yarn-scale model. Meanwhile, the corresponding UMAT subroutine was written to judge the damage initiation and damage evolution process of the material. The damage evolution and failure process of plain woven SiC/SiC composites under uniaxial tension were simulated. The results show that the X-direction tensile stress-strain curve is in good agreement with the experimental curve. The strength properties and damage evolution of plain woven SiC/SiC composites are effectively predicted.

Keywords：multi-scale; plain woven; SiC/SiC; mechanical properties

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Misorientation informed numerical framework for elasto-plastic stress corrosion cracking in polycrystalline materials

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ABSTRACT

Engineering structures often encounter stress corrosion cracking (SCC) leading to their catastrophic failure during in-service conditions. SCC is a coupled chemo-mechanical phenomenon where pit to crack transition occurs under mechanical loading in various chemical milieu. Ultimately, depending on crack driving kinetics, fracture continues to propagate in the structural elements. Several experimental studies have shown the dependence of microstructural features of constituent material such as / including grain sizes and crystallographic texture on the formation of the intricate SCC profile in polycrystalline materials. Specifically, grain boundary misorientation plays a significant role in the trans/inter-granular kinetics of corrosion, as well as in the evolution of fracture. It has been revealed that high angle grain boundaries are more susceptible to inter-granular stress corrosion cracking compared to low angle grain boundaries. Despite numerous experimental and numerical investigations, the influence of grain boundary misorientation angle on corrosion evolution and subsequent emergence of trans/inter-granular fracture is not addressed rigorously. Therefore, the present study aims to build a grain boundary continuum-informed, chemo-mechanically coupled model for corrosion and the subsequent elasto-plastic fracture of a polycrystalline material system.

In the present work, a thermodynamically consistent numerical framework is developed to systematically account for corrosion, inelastic deformation and associated crack initiation and propagation. Phase field methods are adopted to track the interface evolution for corrosion and crack growth in a diffusive manner. Non-equilibrium thermodynamics is employed to extract the constitutive relations and driving forces for the evolution laws of phase field variables. An energy density threshold is introduced to control the onset of damage and ensure elasto-plastic fracture. The influence of crystal orientation and grain boundary misorientation angle is considered in elastic moduli, corrosion kinetic parameter and fracture toughness of the grains and grain boundaries. Finally, employing finite element procedure, the discretized equations are obtained for displacement and phase field variables related to corrosion as well as regularized crack. A systematic parametric study is performed to investigate the role of grain sizes, crystallographic textures and associated grain boundary misorientation angle over the spatial evolution of fracture. Finally, detailed microstructure-informed fracture maps are established under different chemo-mechanical conditions.

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Asymptotic homogenization for the phase field fracture of heterogeneous materials and application to toughening

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ABSTRACT

We propose an asymptotic homogenization framework to account for the fracture of heterogeneous materials; the full text of this work is referred to [1]. This framework assumes that the microscopic fracture behavior is accurately described by the phase field model [2]. With this model, the non-interpenetration constraint is accounted for with a tension-compression split [3]; the irreversibility of crack propagation is enforced with a history variable [4] and the stress criterion for crack nucleation is incorporated with the model of Tanné et al. [5]

By employing asymptotic homogenization [6] on this underlying model, a homogenized model with anisotropic effective properties such as the degraded elasticity tensor and the fracture toughness is derived. Specifically, as the size of the representative volume element at the microscale tends to zero, asymptotic expansions of the displacement and phase fields are performed to obtain a macroscopic model with anisotropic effective elastic tensors and anisotropic effective fracture toughness as material parameters.

The resulting homogenized model not only reproduces the fracture behavior of the original heterogeneous microscopic model but also quantitatively predicts the toughening effect of heterogeneous materials under certain conditions. Specifically, when the fracture toughnesses of all constituents are the same, the toughening effect depends on whether there is a contrast in the toughness moduli of the constituents. Here, the toughness modulus refers to the energy absorbed by each constituent per unit volume before fracture.

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On the Modeling of Quasi-brittle Materials with Analytical-based Micromechanical Formulations

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ABSTRACT

Micromechanical models [1-3] are analytical-based multiscale techniques for the constitutive modeling of quasi-brittle materials. By combining mean-field homogenization and principles of linear fracture mechanics, these models offer the advantage of requiring few input parameters and using internal variables with clear physical meanings.

However, current approaches still struggle to capture complex failure processes and suffer from important pathologies such as i) spurious localization of crack directions ii) inability to correctly capture the asymmetry between tensile and compressive failure iii) unstable or unphysical softening responses iv) and the use of physical models beyond their applicability range; among others.

In this context, this work first critically examines the predictive capabilities of current micromechanical models, highlighting the influence of different homogenization strategies and damage-resistance functions on their behavior and stability. Then, a new model is proposed that employs mean-field techniques to describe the behavior of the damaged material along discretized orientations. An averaging procedure inspired by the Microplane models [4] is applied to obtain an effective macroscopic response from this discretized solution. With this combination, damage evolution is driven by a local strain, akin to the formulation in Ref. [5]. The use of such strain helps produce the desired tensile-compressive asymmetry while also avoiding spurious localization of crack directions.

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Minisymposium QBC:

Quasi-brittle cracking, coupled processes and hydraulic fractures

Organized by G. Xotta, I. Carol and G. Pijaudier-Cabot

A couple fluid-diffusion and elasto-damage model for numerical simulation of hydraulic fracture. – CFRAC 2025

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ABSTRACT

The study of hydraulic fracturing is still an important research topic today for the appropriate use and management of natural resources. This has led to the development of increasingly efficient and accurate numerical models, suitable for the study and analyses on this topic.

The present work aims to develop a coupled fluid diffusion and rock deformation with damage model in order to simulate hydraulic fracture propagation in porous media. In the proposed model, a nonlocal integral-type continuum damage formulation is applied to describe the damage evolution under dynamic excitation. Furthermore, the mathematical representation of the solid is based on Biot's theory and the definition of the effective stress for poro-damage-elasticity, together with generalized Darcy's law for the fluid phase. Through the Galerkin method, the discrete coupled multi-field formulation of the partial differential equations was developed [1]. The numerical solution of the initial-boundary value coupled problem in space was obtained by using the well-known Finite Element Method (FEM) with inf-sup stable discretization while, for temporal integration, one–step generalized trapezoidal method [2]. The fully coupled equations were solved monolithically using a Newton procedure, and the numerical results are validated against available experimental and numerical data.

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Numerical Analysis of Quasi-Brittle Cracking using Enhanced Accuracy Finite Element Technologies

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ABSTRACT

When computing problems of localized structural failure employing the standard displacement-based finite element (FE) formulation from solid mechanics the results in terms of crack trajectories and failure mechanisms have been found to be spuriously dependent on the orientation of the mesh adopted to perform the calculations. Since the first unambiguous reports of this issue in the 1980s, many alternative models for fracture have been proposed attempting to solve it. However, still today, there exists no general consensus as to which is the method that should be used.

This aspect has been addressed by the authors via the adoption of a mixed strain/displacement finite element formulation when computing quasi-brittle cracking. In this FE formulation the independent interpolation of the strain increases the accuracy of the computed solution and guarantees the local convergence of the solution, permitting to obtain mesh bias objective results [1-2]. This represents a fundamental improvement over the standard FE formulation where strains are evaluated as local derivatives of the displacements, and where the local convergence in terms of stresses and strains is not ensured. The enhanced accuracy attained by the mixed formulation in the area of the vicinity of the propagating crack represents a decisive feature for attaining mesh objective results that are not spuriously dependent on the orientation of the FE mesh.

To increase the efficiency of the adopted mixed formulation, an Adaptive Formulation Refinement strategy is employed [3]. This allows to perform the numerical simulations using the standard displacement-based FE formulation and to adaptively switch to the mixed strain/displacement FE only in the regions of the domain where the crack develops while maintaining the standard formulation everywhere else in the structure. This introduces important savings in computational cost while preserving the quality, mesh objectivity and accuracy of the fracture results generated by the mixed formulation. To further increase the cost-efficiency of the calculations, this AFR strategy is employed together with an octree-based Adaptive Mesh Refinement (AMR) strategy. In this manner, the FE mesh is adaptively refined only in the specific areas of the domains where fractures appear, allowing to start the computations with an initially relatively coarse mesh and to subsequently perform several steps of mesh refinement only in the areas cracking occurs.

The accuracy and cost-efficiency of the proposed framework are assessed through a comprehensive set of numerical simulations of benchmark problems and experiments. The computations demonstrate that the framework based on the mixed formulation, combined with the AFR and AMR strategies allows to obtain mesh bias objective results for crack trajectories, collapse mechanisms, load capacity, and nonlinear response. Both 2D and 3D experimental results are accurately replicated.

The comparative assessment of the proposed mixed FE formulation with corresponding computations using alternative methods for fracture is presented, and a critical assessment of alternative methods for quasi-brittle cracking is performed in terms of cost-efficiency, generality, implementation effort and other key aspects.

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Scratch testing for measuring fracture properties of rocks - a computational approach

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Abstract: In geomechanics, hydrocarbon drilling, and geothermal energy, obtaining specimens for fracture testing and determining fracture energy remains a significant challenge. On one hand, classical experiments e.g., on semi-circular notched specimens, are one possibility but size effect tests must be performed to arrive to the fracture energy viewed as a material property. On the other hand, scratch testing offers a promising alternative. Scratch testing can be performed directly on cores obtained during drilling (without destroying them). Yet, interpretation in terms of fracture properties is highly debated. Analytical formulations show that at shallow depths, the cutting force, perpendicular to the cutting surface, correlates with the material compressive strength, while at greater depths, it relates to fracture toughness; however, these formulations lack precision in identifying the transitional depth. Experimental results on several types of rocks highlight the difficulty of capturing the transitional depth between ductile and brittle failure modes, a critical indicator of failure mechanisms. Recent experimental studies suggest that the transition depth is less than 1 mm, though it likely depends on material properties. Definitely, there is a need to further investigate the failure processes involved during scratch testing and this is performed with the help of the Lattice Discrete Particle Model in the present contribution. Our computational results on sandstone reveal that several regimes are observed and the first peak seems directly related to fracture while others might better be attributed to shearing. Fracture, when it happens, occurs through a sequence of cracking events, making the average cutting force an unreliable measure for determining fracture properties. These results provide new insights into material failure mechanisms, focusing on understanding energy dissipation during scratch testing.

Keywords: Scratch testing; lattice models; sandstone; dissipated energy; depth of cut; transitional depth; size effects.

Extension and validation of the microplane-based thermo-hygro-mechanical model to a timber composite connection

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ABSTRACT

In the present research, potentials and limits of using scaled models in timber construction were investigated through experimental and numerical study. With this purpose, a scaled timber composite column-to-slab connection (*model*) was mechanically tested under three-point bending and the results compared with the same test performed on a real-sized connection (*prototype*). The connection is a combination of softwood (spruce) in form of cross-laminated timber (CLT) and hardwood (beech) in form of laminated veneer lumber (LVL). Additionally, the scaled connection was also exposed to cyclic thermal as well cyclic hygral load prior to performing the bending test.

In the numerical study, the previously developed microplane model for wood [1] was used to investigate the scaled connection. To this end it was necessary to further extend the proposed model for wood [1] to realistically represent the multiple fibre orientations in the CLT plate and the LVL insert.

The obtained results for the mechanical test show a good agreement between the experimental and the numerical simulation on the scaled specimens, in terms of load-displacement curve and failure mode. The same failure mode was also observed in the experiments on both the scaled and the real-sized connection. The results indicate that the chosen numerical approach can support the design of novel timber composite systems [2].

Regarding the cyclic environmental tests (hygral and thermal), the model can well reproduce the moisture distribution in the specimens, as well as the moisture-induced cracking due to differential deformations between softwood and hardwood under shrinkage (drying) and swelling (wetting). Another important result is that the cracking observed during the environmental tests (mainly thermal test) has no significant impact on the mechanical response of the connection.

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Calibration and validation of the coupled microplane-based thermo-hygro-mechanical model for clear wood

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ABSTRACT

Wood is one of the oldest building materials, owing to its availability, versatility and durability. In the modern building industry, timber products play an important role with respect to sustainability and resource management. The fact that wood is a natural material with inherent defects such as knots and cracks, very high variability between different types of wood and high scatter typical of natural materials poses a great challenge. Unlike other building materials, wood exhibits orthotropic behaviour with very different response in the three relevant directions. The orthotropic nature is reflected not only in mechanical but also in the hygral and thermal response. Additionally, the fact that mechanical properties of wood are highly dependent on the moisture content, type of wood (early wood vs. late wood) and the natural geometry of the individual trunks (year rings thickness) makes the assessment of material behaviour and structural response even more complex. In spite of the more than one century of material testing on wood, many aspects of the behaviour have not been sufficiently addressed yet.

Suitable numerical models can be used to understand the complex behaviour of wood and structural timber. The main prerequisite for a realistic and reliable numerical analysis is the understanding of the mechanical behaviour at material level as well as the thermal and hygral performance of the material. Full description of all aspects of material behaviour is currently not available from the literature.

Therefore, in the present work, the recently developed microplane framework for clear wood is calibrated and validated based on experimental results on two different wood types, namely spruce (softwood) and oak (hardwood). In the first part, the mechanical behaviour (uniaxial tension and compression) in three main material directions (parallel to grain, orthogonal to grain with differentiation between radial and tangential direction) using small samples almost free of defects (clear wood) is investigated. These results provided input for the numerical analysis in form of complete stress-strain curves. Second part of the study deals with thermal and hygral behaviour of wood as well as their coupling with the mechanical response. The experiments include the estimation of absorption-desorption curves and estimation of thermal and hygral deformations in the three material directions. These data are used to calibrate the numerical model with respect to shrinkage and swelling coefficients. The final experimental series included cyclic thermal and cyclic hygral tests, which were used to validate the model. It was found that the numerical model can realistically reproduce the hygral and thermal deformations of the material. This study was the starting point for the extension of the model to capture the behaviour of various timber composite systems, which may include combinations (glued or otherwise connected) of soft- and hardwood.

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A phase-field framework to model crack propagation in layered poroelastic media with weak interfaces.

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ABSTRACT

We present a phase-field framework to model crack propagation in layered poroelastic media with weak interfaces. The proposed approach employs a three-field formulation with displacements, pressure, and damage as the primary field variables, governed by the equations of linear momentum balance, mass balance, and damage evolution. The constitutive response of the medium is modeled as per Biot's theory of linear poroelasticity. A novel pressure history field variable is proposed to extend the hybrid phase-field method of Ambati et al. (2015) to model crack propagation in poroelastic materials. This pressure history field prevents non-physical behavior, including (a) negative damage, (b) damage exceeding 1, and (c) reversible damage when modeling crack propagation in poroelastic materials. These issues arise because the history field variable in the standard approach is designed for purely mechanical problems and did not include the additional contributions from the pressure. Additionally, we also provide a means to incorporate weak interface effects including both debonding and slip, within a phase-field framework and apply the resulting model to study fluid-driven crack propagation in layered media with frictional interfaces. Interface debonding is incorporated by adding interface terms to the elastic and crack surface energy by evaluating an additional line integral (surface integral in 3D) at material interfaces. Interface slip is incorporated by modifying the stress tensor within a regularized interface region of the phase- field formulation, based on Fei and Choo (2020). The method effectively identifies contact conditions, such as stick-slip behavior, and enforces no-penetration constraints along the interface. To demonstrate the performance of the proposed formulation, we validated it against several benchmark problems, with results showing good agreement with existing studies. The proposed framework provides a robust tool for simulating fluid-driven fracture in complex layered poroelastic systems.

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Fluid-induced fracture by CO_2 injection in a partially-saturated deep saline aquifer

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ABSTRACT

CO_2 storage in deep saline aquifers poses a number of technical challenges including the possibility of rock fracture near the wellbore. This phenomenon is studied with a fully-coupled THGM FE model using zero-thickness interface elements [1]. The water retention curve (WRC) used for the continuum medium is the well-known van Genuchten model and, in the case of interfaces, a modified version which includes a reduction factor of the WRC parameters is considered [2]. CO_2 is modeled as a pure non-ideal gas using the Peng-Robinson equation of state as proposed in the literature [3], CO_2 dissolution in the liquid phase is considered using Henry's Law and is a requirement for modeling the initial situation of full liquid saturation.

The case analyzed consists of a horizontal section of a layer of a partially-saturated aquifer with a single closed fracture pre-inserted in the center of the domain connecting the CO_2 injection wellbore with the opposite boundary. An analysis of the sensitivity of the results to the initial saturation degree, permeability of the aquifer and mechanical parameters of the interface is presented. Results obtained indicate that CO_2 injection in an initially fully-saturated aquifer leads to higher fluid pressures that depending on injection rate may cause crack initiation and propagation. This induced fracture changes the flow pattern and the well injectivity in time. Thermal effect could accelerate the induced fracture propagation.

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On the modelling of fluid and ion transport through cracks in quasi-brittle materials in multiphysics phase-field-based models

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ABSTRACT

The transport of liquids, gases and dissolved ionic species through cracks in quasi-brittle materials plays a critical role in many practical applications. The transport of pressurised liquids and gases through a cracking geological medium is used to extract oil, gas and geothermal energy or to sequester carbon dioxide. Water and aggressive ionic species are transported through variably saturated surface cracks in reinforced concrete, rapidly accelerating corrosion initiation and hence compromising concrete durability. The modelling of crack transport is therefore crucial when performing multiphysics numerical simulations of the phenomena described above. In recent years, phase-field fracture models have gained remarkable popularity due to their numerical robustness and ability to capture complex cracking patterns. To simulate the enhanced transport through cracks compared to the undamaged bulk material, the phase-field variable ϕ, which indicates material damage, can be conveniently coupled to transport properties such as water permeability or ionic diffusivity. For example, studies coupling the phase-field fracture model with diffusion-driven transport in concrete mostly assume a power function interpolation of the diffusivity $D = (1-\phi)^m D_c + \phi^m D_L$ between the initial uncracked concrete diffusivity D_C and the diffusivity in liquid D_L, typically choosing $m = 1$. While it is well documented experimentally that the flux of transported medium through the crack is strongly affected by crack width, phase-field fracture models do not directly provide crack opening, and it has been unclear whether the power function interpolation approach leads to an accurate dependence of the flux of diffusing species on crack width. To elucidate this matter, we focus on the diffusion of chlorides in cracked concrete, the mechanical behaviour of which is described by the quasi-brittle fracture model. Results indicate that the currently popular power function interpolation approach greatly overestimates the flux of chlorides through the crack compared to experimental results and can even lead to an unphysical decrease in the average diffusivity through the crack. Also, it is found that the power function interpolation approach does not allow to consider that up to a certain crack width, the diffusive properties of the concrete remain unchanged, whereas for large cracks the diffusivity no longer increases above D_L. To correct these discrepancies, a distinction is made between the physical diffusivity D and the numerical diffusivity in the crack D_N. A new simple algorithm is proposed that allows the calculation of an appropriate function $D_N = f(\phi)$ for a given quasi-brittle phase-field model, material mechanical properties and characteristic phase-field length scale, so that the experimentally measured dependence of flux on crack width is recovered for arbitrary softening. The application of the proposed algorithm is showcased on the examples of chloride diffusion and water convection in cracked concrete, demonstrating its applicability to different transport regimes, including hydraulic fracture. The numerical sensitivity of the algorithm is investigated, showing, among other things, a very low sensitivity to the number of steps of the proposed method.

Improved interface material model for simulating cracking, shearing and crushing in unreinforced masonry structures subjected to cyclic loading

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ABSTRACT

The vast majority of the European architectural heritage and a large part of old dwellings consist of masonry. Among these structures, unreinforced masonry buildings are particularly vulnerable to both mechanical and environmental actions.

Several modelling approaches have been developed and applied to the simulation of the structural response of these masonry buildings. The simplified micromodelling approach is one of them, where the bricks are represented by continuum elements with elastic material properties, while all inelastic behaviour is concentrated in zero-thickness interfaces between the bricks [1]. This approach provides a good balance between accuracy and computational efficiency; however, modeling all failure modes within these interfaces can pose significant challenges to the numerical algorithm's robustness, particularly under complex cyclic loading conditions.

In this work, a recent interface material model, originally developed in the context of Discrete Element Method [2], has been improved and implemented in an implicit Finite Element Code. The interface accounts for mixed-mode fracture in tension-shearing and combines de-cohesion and friction in compression-shearing. The robustness of the model has been improved by regularizing the frictional contribution. For use in implicit analyses, the consistent tangent stiffness has been derived in order to efficiently simulate the evolution of damage under monotonic and cyclic loading. Furthermore, the model has been extended with a plastic-damage cap to capture the crushing behaviour of the material.

The improved interface model has been validated against full-scale laboratory tests of walls and a spandrel subjected to both monotonic and cyclic loading, demonstrating satisfactory results in replicating various failure mechanisms and the unloading–reloading response of masonry.

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Phase-field Modelling of Desiccation Cracks: Influence of Crack Resolution on Coupled Behavior

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ABSTRACT

Multi-physics models play a crucial role in simulating coupled processes such as drying-induced cracking, particularly relevant in applications such as radioactive waste disposal, where understanding crack behavior for predicting the long-term stability and integrity of the waste containment in geological and geotechnical systems is vital. In Cajuhi et al. [1] a hydro-mechanical framework combined with the phase-field approach for modeling desiccation cracking in Opalinus Clay has been proposed and tested at in-situ scale. A key parameter in phase-field models is the length scale, which governs the spatial resolution of damage zones. The length scale also influences the mesh resolution, with smaller values requiring finer mesh elements. The length scale was determined based on experimental parameters in [1]. The current study explores how variations in the length scale parameter affect the hydraulic, mechanical, and hydro-mechanical responses, particularly with respect to crack initiation, depth of propagation, and fracture localization within rock formations. Through numerical simulations, we investigate the impact of the length scale on desiccation cracking in Opalinus Clay. Our findings highlight the sensitivity of crack onset, damage zone localization, and energy dissipation to this parameter. The results underscore the trade-offs between computational efficiency and physical accuracy, offering insights for calibrating the length scale in practical applications. These insights are relevant for optimizing models used in the context of radioactive waste disposal and in understanding fracture behavior in geological systems.

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Volume expansion vs cryosuction in frost-driven fracture: a look through numerical modelling

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ABSTRACT

Exposing wet solids to cold environments can cause the liquid imbued within to freeze. Far from innocuous, the presence of these internally growing ice inclusions can greatly compromise the solid's structural integrity as it has the potential to trigger fracture. Traditionally, the volume expansion of water upon freezing has been assumed to be the leading factor causing frost-driven fracture in wet solids. This classical line of thought hypothesizes that the increased volume of ice has to be accommodated by the permeable solid's microstructure, hence causing it to stretch and eventually rupture. However, conclusive experimental evidence shows that frost-driven fracture can also occur in wet solids imbued with liquids that contract upon freezing [1], hence ruling out this physical process as the sole cause. Instead, another physical mechanism has recently arisen as a contender for causing frost-driven fracture: cryosuction [2]. This concept stands for the migration of liquid water towards the ice front due to a reduction of the liquid pressure therein. As such, cryosuction can potentially play a dual role in frost-driven fracture: (i) leading to cracking by desiccation, and (ii) allowing ice to build up within the internal crevices for as long as the supply of supercooled water holds.

In this context, the present work leverages numerical models inspired by experimental evidence to weigh the contribution of these two mechanisms to the occurrence of frost-driven fracture, using hydrogels as a model for wet solids. This is done through two different approaches. Firstly, a simplified hyperelastic numerical model is used to assess the difference between the actual freezing experiments and the purely mechanical deformation required for the hydrogel to accommodate the experimentally documented ice topology, hence providing an indirect quantification of the actual cryosuction-induced hydrogel desiccation around the ice-filled crack tip. Secondly, a hygro-mechanical numerical model of the hydrogel is set up to preliminarily describe the migration of water towards the ice-filled crack as it grows in time at different speeds. As in the previous model, the crack shape is directly extracted from the experimental observations, while the liquid pressure drop at the crack lips is derived from the ice-water thermodynamic equilibrium. This model provides detailed insights into how cryosuction draws water from the bulk as the ice-filled crack grows, and it helps interpret the experimentally observed size-dependency of the desiccation-affected region near the ice-filled cracks.

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Towards large scale simulations of fibre reinforced concrete wave energy converters

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ABSTRACT

Wave energy converters (WEC) are one of the modern systems which produce clean energy from the sea waves. Due to very harsh marine environmental conditions, exceptional performance of the structural elements of WECs is required. By default, the WEC floater hulls are made from steel or aluminium, but these materials can be replaced by high performance concrete (HPC). In order to fulfil carbon footprint reduction sustainability goals, this concrete is developed with high cement replacement ratio by alternative binders. By adding fibres to HPC the ductility after cracking is significantly increased and fibre reinforced high performance concrete (FRHPC) is formed.

The numerical description of concrete made floater in the marine environment is a very challenging task. The first difficulty comes from the material itself. The behaviour of plain concrete is very complex and this complexity is mainly manifested by the presence of cracks. With fibres inside the concrete, some extra failure modes have to be also properly captured. There are two main numerical approaches to handle fibre reinforced concrete (FRC). In the first method, the behaviour of plain concrete is independently described and explicit definition of fibres is included in the model [1]. Between concrete and fibres, advanced (slip) or relatively simple (fix) conditions are implied. Alternatively, FRC is treated as a homogeneous material and an overall (averaged) response is derived [2]. The second challenge comes from the size of the geometry analysed, which enforces a balance between the accuracy of the material formulation and overall specimen performance.

The intention of the paper is to present result of numerical simulations of a concrete WEC scaled prototype subjected to loads from the marine environment. In the first step, small specimens will analysed and the material model with explicit fibres derived in [1] will be used. In parallel, a homogeneous equivalent description of FRHPC will be proposed and the obtained results will be compared. The influence of selected parameters (e.g. fibres content) and methods how to describe them will be analysed. The special attention will be paid to the potential orthogonality of the material characteristic enforced by application of FRC to thin walls. Then equivalent constitutive law will be used to simulate the performance of large size WEC prototype. For critical sections, detailed simulations with explicit fibres will be done.

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A Discrete Approach to Fracture Modeling in Reinforced Concrete: Application to Size Effect Analysis in RC Beams

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ABSTRACT

This work introduces a computational model developed in [1] for simulating the fracture behavior of reinforced concrete. Cracks are discretely modeled using zero-thickness cohesive interface elements, while the reinforcement is explicitly represented by elastoplastic Timoshenko beam elements. The cohesive-frictional interaction between reinforcement and concrete is modeled via coupling elements, conceptualized as elastoplastic bedding between the concrete and reinforcement phases.

To demonstrate the performance of the proposed model, two series of experiments on reinforced concrete beams without shear reinforcement subjected to four-point bending were numerically analyzed in a 3D setting. In the first series of tests performed by Syroka-Korol and Tejchman [2], the beam size was scaled in two dimensions. A distinct feature of these tests is that the shear failure mode, featuring a critical diagonal crack, was consistent across all sizes, enabling assessment of the proposed model to capture size-effect. In the second series by Suchorzewski et al. [3], only the beam depth was scaled. This series exhibited markedly different failure modes for each size, allowing the assessment of the capabilities of the proposed modeling approach to capture the effects of the shape and size on the mechanical response of reinforced concrete beams.

The proposed model has demonstrated its capability to reproduce the peak loads, different failure modes and crack patterns in all structural experiments, which makes it a suitable tool for both serviceability and failure analysis of RC structures. The presentation concludes by discussing the sensitivity of the proposed model to individual parameters and their influence on capturing failure mechanisms in reinforced concrete.

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Localization Properties of Damage-Plastic Model for Concrete Under General Stress States

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ABSTRACT

Early models for concrete failure were often limited in scope, focusing, e.g., only on tensile-dominated cracking. Perhaps the most flexible formulation can be obtained by combining damage with plasticity. Such models are sometimes presented as damage enriched by permanent strain and sometimes as plasticity with degrading elastic stiffness. One widely used model of this kind was proposed by Grassl and Jirásek [1] and later extended and modified by Grassl et al. [2].

In this contribution, localization properties of the damage-plastic model for concrete will be explored in detail, using the standard criterion based on the eigenvalues of the acoustic tensor deduced from the material tangent stiffness tensor. The analysis should identify the necessary conditions for the onset of formation of localized bands, after which the standard local formulation of the model ceases to provide objective description of the failure process and some form of regularization is needed. The problem is interesting and challenging due to multiple potential sources of instabilities – softening and nonassociated plastic flow. Attention will be focused on localization under shear or compression, including confined compression, which is much less understood that the usual tensile cracking. Differences between the original formulation with a single damage variable and the modified formulation with separate tensile and compressive damage will be examined. Consequences for computational modeling of general concrete failure and possible regularization techniques will be discussed.

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Simulation of the Gap Test and Implications for Model Calibration

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ABSTRACT

Fracture properties of concrete are often characterized by traction-separation laws with softening, which describe the behavior of a fictitious cohesive crack that approximately replaces the localized fracture process zone. The area under the cohesive diagram is interpreted as the fracture energy and is often deduced from fracture tests in which the material is in a state close to uniaxial tension. Recently, Bažant, Cusatis and coworkers [1-2] have demonstrated experimentally that the dissipated energy per unit area of the crack and thus the entire cohesive curve are strongly affected by stresses parallel to the crack. Numerical investigations have shown that this is not always properly captured by existing constitutive models for concrete.

In this contribution, the so-called gap test [1-2] will be simulated using simple damage models and also the damage-plastic model originally proposed by Grassl and Jirásek [3] and later extended and modified by Grassl et al. [4]. The results will be critically evaluated and model parameters that control the sensitivity of the fracture process to the crack-parallel stresses will be identified. Implications for the structure of the constitutive model will be discussed and a parameter identification procedure will be developed. Finally, the efficiency and accuracy of the technique based on adjustment of certain parameters depending on the size of finite elements will be evaluated, and alternative regularization techniques that eliminate pathological mesh sensitivity will be tested.

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Minisymposium RFM:

Theoretical and numerical aspects of regularized failure models: Phase-field and other models

Organized by L. de Lorenzis, M. Jirásek, C. Maurini and N. Moës

Crack Driving Force and Post-fracture Behavior within the Phase-field Approach – a Comparative Study on Energetic Splits

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ABSTRACT

The phase-field approach has attracted great attention in the numerical modeling of fracture, including nucleation, propagation, branching and merging. With great endeavors from many researchers, the phase-field theory has been intensively investigated and greatly extended into different fracture problems. Amongst the many important issues within phase-field fracture, the energetic decomposition/split, that directly influences the crack driving force, is a non-trivial aspect and still remains an active research topic.

In this work, we focus on a comparative study between two interesting phase-field split models, i.e. the Representative Crack Element (RCE) approach [1] and the Star-convex approach [2]. By employing phase-field degradation as the interpolation weight, the RCE model combines a discrete crack description for the damaged state and a continuous description for the intact state. On the other hand, the Star-convex model extends the volumetric-deviatoric (VD) split with an additional parameter. In general, both models could describe tension-compression asymmetric failure.

Within the current study [3], analytical aspects of the interested models are firstly discussed. This includes a one-dimensional discussion for crack opening and closing condition, and a multi-dimensional elastic domain identification. Further characteristics that are of our interest include post-fracture behavior, mixed-mode cracking and compression induced cracking. For these aspects, several numerical benchmarks are considered within the context of the finite element method, together with reference from analytical solutions and/or experiments.

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On the existence of a regularization length scale in fracture

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ABSTRACT

The talk explores the physical existence of the regularization length scale employed in diffuse fracture models. It begins with macroscopic examples where conventional linear elastic fracture mechanics fail to produce realistic predictions. We address all three fundamental fracture modes: the size effect in tensile opening, the branching angle in in-plane shear [1], and echelon cracking in antiplane shear [2].

Next, we focus on identifying this length scale in amorphous silica through atomic-scale investigations. Our study reveals distinct energy contributions during fracture, successfully differentiating between free surface energy and fracture surface energy. Importantly, we demonstrate that even in ideally brittle materials, like glasses, diffuse damage is indispensable during the creation of a new surface.

These findings highlight that diffuse damage contributes significantly to fracture toughness in most materials. As a result, the study provides a robust physical foundation for the regularization length scale employed in phase-field models of fracture.

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An high order AT1 phase-field model for brittle fracture

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ABSTRACT

A key aspect of phase-field modeling, based on the variational formulation of brittle fracture, is the accurate representation of the surface energy dissipation during the fracture process. From a mechanical standpoint, AT1 functionals typically exhibit better properties than AT2, as they result in a clear linear elastic regime before the onset of fracture [1]. Moreover, for given values of internal length and mesh size the damage profile around the crack is usually narrower with AT1. High-order functionals, while offering similar accuracy to low-order ones, allow for larger mesh sizes in discretization, offsetting the computational costs associated with second-order derivatives [2]. In [3] we aim to combine these advantages by proposing a novel fourth-order AT1 phase-field model for brittle fracture within an isogeometric framework, which provides a straightforward discretization of the high-order term in the fracture energy functional. We first establish a Γ-convergence result for the AT1 functional (in both the continuum and discretized isogeometric settings) through a detailed analysis of the optimal transition profile, which ultimately provides an explicit correction factor for toughness and determines the exact size of the transition region. Previous results in the literature, see e.g. [4, 5] do not apply here due to the combination of the high order term and the constraint that the phase-field variable must take values between 0 and 1. Hence, we developed a novel line of proof that is quite general and applies also to the other AT1 functionals in the literature. The talk will primarily focus on this theoretical part, which in the paper is complemented by a detailed study of the model's numerical performance. As expected, the simulations show that the proposed fourth-order AT1 model outperforms the lower-order AT1 and AT2 models in accuracy, while enabling the use of larger mesh sizes and reducing computational cost.

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On the energy decomposition of anisotropic materials in variational phase-field fracture models

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ABSTRACT

Anisotropy is a fundamental property of many materials, arising either from their manufacturing processes or inherent microstructures. This directional dependence can significantly influence the material's failure behavior. To understand material deformation and failure, it is essential to decompose the strain energy density into its distortional and dilatational components. Different materials exhibit distinct responses to these types of deformations. For instance, metals typically withstand higher shear strains before failure, whereas ceramics are more prone to damage from volumetric changes. By decomposing the strain energy, engineers can apply appropriate theories and models to accurately predict and analyze material behavior under complex loading conditions.

Phase-field fracture models have achieved significant success in recent years and are increasingly emerging as the dominant approach for understanding and predicting materials failure. The additive decomposition of strain energy plays a pivotal role in the development of these methods, influencing both the nucleation and propagation of cracks. For isotropic materials, the spherical and deviatoric stress components are work-conjugate to the volumetric and isochoric strain components, respectively. This decomposition reflects the inherent symmetries of isotropic materials. Consequently, it is not applicable to anisotropic materials, except in cases where their symmetries align with those of isotropic materials. In this work, we introduce two energy decomposition approaches—direct and indirect—that preserve the orthogonality condition for arbitrary anisotropic materials. Through representative numerical examples, we evaluate and compare the characteristics of these two decompositions.

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Working towards a modular, fully-coupled phase field fracture model integrating elasticity, plasticity, and damage

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Abstract

Many phase field fracture models that have been implemented to date are opinionated regarding the choice of elastic model, plastic model, damage model, etc. While this enables easier development of the formulation itself, the resulting model is inflexible and often only applies to a subset of problems of interest. Further, if a change in model is desired, it may be required to redo much of the derivation and implementation. This work aims to develop and implement a generalized, variational, fully-coupled, and modular phase field fracture formulation capable of handling a diverse range of problems. The choices of elastic model, plastic model, damage model, rate-(in)dependence, degradation functions, and tension-compression split are all modularized with well-developed interfaces, enabling the development of solver infrastructure independent from the particular choices of models. While this approach brings its own challenges, it also enables classes of models which were previously tedious to implement, thus allowing the exploration of more complex problems.

In this presentation, we detail this modular approach from analytical derivations through to implementation in SIERRA, a robust multi-physical finite element code developed at Sandia National Laboratories. The approach will be demonstrated for several canonical model forms, including elastic and elastic-plastic fracture mechanics.

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A variational damage-plasticity model at finite strains

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ABSTRACT

The consideration of ductile fracture at finite strains involves different challenges, such as accounting for large deformations, geometric non-linearities and the coupling of damage and plasticity. This work aims to develop a variational damage-plasticity model at finite strains with damage represented by a phase-field variable. The coupled damage-plasticity problem is formulated in the framework of rate-independent problems, where it is represented by a stored energy functional and a dissipation potential [1].

Solutions of the variational formulation are obtained by considering a natural time discretisation, which leads to a sequence of minimisation problems to be solved. The formulation as a rate-independent system in the sense of [1] allows the construction of a numerical solver based on a proximal Newton method coupled with robust and efficient multigrid methods. This approach, which can be applied to different plasticity models, ensures convergence, replaces the classical predictor-corrector scheme for the plastic strain, and offers a reduced computation time [2].

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A variational model coupling cavitation and damage for fracture in nearly incompressible materials

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ABSTRACT

Variational phase-field models for brittle fracture are widely used due to their ability to reproduce complex crack patterns without the need for ad hoc criteria [1] and to effectively handle crack nucleation under tensile loading [2]. However, the treatment of crack nucleation under multi-axial stress states in phase-field models remains a topic of active discussion, with several unresolved challenges. Among these challenges are the inability to flexibly define the crack nucleation criterion under multi-axial stress states and the difficulty of modelling crack nucleation in materials approaching the incompressibility limit. In this contribution, we focus on the issue of crack nucleation in nearly incompressible materials, with particular attention to the well-known poker-chip test introduced by Gent and Lindley [3]. We propose a novel phase-field model coupled with a nonlinear model describing cavitation at the macroscopic level. The nonlinear cavitation model describes two phases: the first phase captures the material's behaviour when it is nearly incompressible and undergoes minimal deformation until the cavitation threshold is reached, while the second phase reflects a nonlinear response caused by the presence of bubbles in the material. These bubbles lead to the loss of the material's nearly incompressible nature, enabling expansion. We combine this macroscopic cavitation model with a variational phase-field model in which the scalar damage variable influences the cavitation threshold. The variation of the cavitation threshold with the damage thus becomes the new variational driving force. In this way, we capture the key features of cavitation and fracture processes in nearly incompressible materials, relying solely on energy minimization and remaining within the variational framework without using ad hoc criteria and non-variational driving forces.

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A Variational Gradient Plasticity Model allowing for Shear Band Localization

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ABSTRACT

Plasticity in nonlinear solid mechanics describes the development of inelastic deformations in engineering materials when a critical stress threshold is exceeded. Experimental observations at the microstructural scale have demonstrated that plastic behaviour depends on grain size, a phenomenon that classical plasticity theories fail to capture due to the absence of an intrinsic material length scale [1]. To address this limitation, we introduce a variational gradient plasticity model incorporating non-local first-order terms, specifically the curl of the plastic strain field, which provides a homogenized measure of dislocation distributions and internal lattice incompatibilities.

Unlike traditional gradient plasticity models that employ quadratic regularization terms to smooth plastic strain gradients, our approach replaces this with a sub-quadratic term that introduces threshold effects, fundamentally altering the plastic response (see [2] and [3]). This novel formulation influences the plastic threshold and enhances the representation of shear band formation by enabling sharper localization effects rather than diffusive smoothing. The impact of these modifications is analyzed through a two-dimensional shear problem involving a hollow cylinder, where both analytical and numerical solutions illustrate the role of first- and second-order curl terms in plastic evolution.

By emphasizing dislocation interactions and their role in plastic localization, this study provides a new framework for modeling size-dependent plasticity with greater fidelity. The proposed approach offers fresh insights into dislocation nucleation, defect formation, and the evolution of curved plastic zones, paving the way for more accurate descriptions of material behavior under extreme conditions.

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On sharp-interface cohesive models with non–linear elastic bulk energy

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ABSTRACT

This study investigates the challenge of unrealistic stress predictions that arise when associating cohesive interface energy with standard linear elasticity, building upon findings in [1]. We focus on anti-plane elasticity under mode III loading, leveraging the Linear Elastic Fracture Mechanics (LEFM) solution [2]. The traditional approach can lead to situations where predicted stress components exceed the fracture strength of the material.

To address this, we incorporate a relaxed bulk energy approach from [3]. This approach utilizes a quadratic law for small strains, transitioning to linear growth upon reaching a critical strain threshold specific to the material. This modification ensures a well-posed problem, paving the way for a viable solution.

We validate our approach through numerical simulations showcasing crack nucleation and propagation along a predefined path. The results show adherence to the stress yield condition, supporting the effectiveness of our methodology in overcoming the limitations of the traditional approach.

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Strength-based phase-field approach to cohesive fracture

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ABSTRACT

The critical stress required to nucleate a crack in a pristine material (the strength) and the energy needed to propagate it (the fracture toughness) are fundamental properties in fracture mechanics. Cohesive-fracture models and gradient damage models have successfully captured these key aspects but exhibit distinct limitations. Cohesive-fracture models with sharp interfaces often face mathematical and numerical challenges when the crack path evolves freely. Conversely, formulating damage models that accommodate arbitrary strength surfaces under multi-axial loading while adhering to Griffith's criterion for crack propagation remains a significant challenge [1-3].

In this work, we propose a novel variational framework for phase-field fracture models with a strength-based formulation. We define undamaged energies with linear growth at infinity and allowing the damage (or phase-field) variable to modulate its slope. This approach explicitly incorporates a strength criterion into the model while maintaining consistency with Griffith's criterion for crack propagation.

We detail the application of this method in the context of antiplane shear and introduce an innovative numerical solution scheme leveraging convex optimization tools. Finally, we outline the extension of this approach to three-dimensional cases.

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A geometrically exact phase field approach to cohesive fracture

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ABSTRACT

Cohesive zone models offer a promising framework for modelling non-linear fracture. In contrast to brittle fracture, where the crack energy is constant, cohesive zone models assume an energy depending on the crack opening. This energy, in turn, leads to a traction-separation law, which describes the traction over the opening of the crack.

Regarding the finite element approximation of fracture, two different approaches can be found. The first class models the crack as a sharp interface, which can be represented using interface elements or by incorporating sharp interfaces within elements (e.g., XFEM). By way of contrast, the second approach approximates the crack surface as diffuse/smeared, resulting in a finite interface thickness. The phase field method offers such a diffuse approximation through the use of an additional order field.

A promising phase field approach to cohesive fracture was introduced by Conti et al. [1] and has since been further developed (e.g., [2,3,4]). This approach is supported by a proven Gamma-convergence and requires only the two field variables: displacement field and order parameter. In this talk, the phase field model of cohesive fracture will be extended to a finite strain framework. Additionally, the MCR effect, which restricts crack evolution to tensile states will be introduced.

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One-Dimensional Comparative Study of the Lip-Field and Phase-Field Formulations for Cohesive Fracture

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ABSTRACT

Developing numerical models for structures made of softening materials remains a challenging research topic. Continuum models within the framework of damage mechanics are commonly used for this purpose. However, as the material softens, the solution to the equilibrium problem becomes non-unique, leading to a pathological dependence on the finite element mesh. To address this issue, several "non-local" formulations have been proposed in the literature. These methods introduce a characteristic length into the numerical formulation. In the last few decades, the Phase-Field variational approach to fracture [1,2] has gained popularity. In this approach, the solution to the damage mechanics problem is obtained by minimizing an incremental energy potential, which is the sum of the elastic energy potential and an energy dissipation potential. Regularization is introduced by adding terms that depend on the gradient of the damage field in the second energy contribution. More recently, [3] proposed a new approach to prevent spurious damage localization: the Lipschitz formulation. In this case, the minimized potential remains purely local, and regularization is achieved by enforcing a Lipschitz regularity constraint on the damage field. This constraint naturally incorporates the characteristic length into the formulation. Moreover, by constructing upper and lower damage bounds that satisfy the Lipschitz constraint, the Lip-Field method can be designed to be non-local within sub-zones, significantly reducing computation time compared to other non-local approaches. Focusing on cohesive fracture [4], this study compares this new regularization method with the Phase-Field model in terms of regularization properties, robustness, and computational cost. Several one-dimensional finite element implementations using alternated minimization solvers are proposed. In particular, after comparing two standard implementations of these approaches, alternative implementations of both methods are developed to reduce computation times, decrease the number of iterations required for convergence, and improve overall convergence.

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Damage of civil engineering works submitted to thermomechanical loading: modelling strategies, achievements and pending questions

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ABSTRACT

Assessing the safety and predicting the lifespan of large-scale civil works involved in electricity generation may advantageously benefit from numerical simulations of concrete damage initiation and propagation. Nevertheless, the need for reliable results and robust and efficient numerical strategies still raises several challenging questions.

When considering individual structural cracks, the limitations of local damage models related to strain-softening have long been established and mature alternatives have emerged, in particular cohesive zone models and nonlocal damage models. However, the former encounter theoretical and numerical difficulties in predicting the crack path while the latter rely on relatively small internal lengths related to the aggregate/cement microstructures, hence resulting in (very) fine meshes and time-consuming computations. To bridge the gap between both, a phase-field regularised cohesive zone model has been proposed in [1], sometimes named length scale insensitive phase-field model since then: it retains the flavour of (gradient-enhanced) nonlocal damage models except for the internal length which is now a numerical parameter; when it goes to zero, the model tends to a cohesive law.

Several complementary topics deserve a close attention. First, the isotropic spectral split between tensile and compressive strain is revisited. It fulfils minimal requirements relative to fracture and provides an interesting contrast between strain-driven and stress-driven shear, but it may exhibit spurious stresses in case of large opening combined with shear. Besides, a supplementary damage mechanism is taken into account in order to limit compressive stresses. Finally, a viscous regularisation is introduced to ensure a time-continuous response of the damage field, a key feature for numerical robustness and reliability [2]. It enables the use of a monolithic solution algorithm in combination with a strict and objective convergence criterion.

The capabilities of this comprehensive modelling strategy are demonstrated in particular by means of a validation test for which experimental results are available. It consists of a reinforced beam submitted to a transient thermal loading (heating of the lower face) followed by four-point bending up to the development of plasticity in the reinforcement frames.

However, in the context of large reinforced concrete structures, many individual cracks are expected, so that the former strategy which consists in modelling each individual crack may lead to hugely expensive computations. An alternative would consist in grouping several cracks together, through a homogenisation scheme for instance, hence reaching a larger scale. Unfortunately, it usually ends up with local constitutive laws that suffer from localisation, hence resulting in ill-posed problems. In our opinion, this is a critical question still open to debate.

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Strongly thermo-mechanically coupled gradient-enhanced damage simulation using the neighbored element method

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ABSTRACT

Temperature has a severe influence on the damaging of structures: materials may possess lower yield strength at higher temperatures, but also thermally induced stresses due to large temperature gradients can cause damage even without mechanical loads. In return, damaged zones change the local material properties yielding a change of the heat transfer and the evolution of the temperature field in general. These coupling effects are especially relevant for thermal shock processes.

Thus, we propose a strongly coupled formulation derived from Hamilton's principle of least action including mechanical equilibrium, heat transfer, and gradient-enhanced damage: the temperature field influences the mechanical equilibrium due to thermal expansion, but also generation of heat due to elastic deformation is explored. Damage due to mechanical loading and the influence of increased heat on the yield limit are included in our model, as well as dissipative heat generation during damage evolution and the influence of varying thermal conductivity in damaged zones.

For a most numerical efficient solution for small time increments, we impose the Neighbored Element Method (NEM): herein, the governing partial differential equation are solved in a staggered manner and the displacement field resulting from the mechanical equilibrium is solved via a Finite Element Approach whereas the heat transfer and damage evolution are solved via a Finite Difference scheme between elements of the mesh.

Several two- and three dimensional numerical examples are shown to demonstrate the robustness and efficiency of the proposed method.

Simulation of crack surface friction within the phase-field method

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ABSTRACT

Cracks and the associated frictional forces that arise under combined compressive and shear loads at the crack surfaces can significantly impact the material behaviour, which is particularly relevant if the load direction changes after the formation of the cracks.

The phase-field method is a powerful method for the simulation of cracks and their propagation, enabling automatic handling of crack propagation, including the detection of the direction and length of the propagation, and it can even capture coalescence and branching of cracks. However, to the best of the author's knowledge, no generalisable method for the simulation of crack surface friction under combined compressive and shear loads within the phase-field method has been published yet. This contribution can therefore be considered as a first attempt in this direction.

Since the cracks are not modelled discretely in the phase-field method, but are represented by a reduction of the material stiffness, which is applied in a certain width that is determined by the internal length parameter, this represents a particular challenge.

Coulomb's friction law is used for the simulation of crack surface friction, and it is adapted for the calculation of the stick and slip state analogously to elastoplastic models.

The method has been tested with a set of numerical tests showing promising results indicating that the approach has the potential to correctly represent crack surface friction in rather general cases. Thus the approach can be a valuable contribution to a more accurate modeling of material behaviour and failure within the framework of the phase-field method.

An effective strategy for modelling sharp bimaterial interfaces in peridynamic models

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ABSTRACT

Increasing structural reliability requires the development of models capable of accurately simulating the mechanical behaviour of structures even in the presence of defects such as voids, inclusions or cracks. Peridynamics, a non-local continuum theory based on an integral formulation, is able to model crack initiation and propagation in solids [1]. It has been successfully used to simulate a variety of damage propagation phenomena, unfortunately due to the non-locality, peridynamic models suffer from two interconnected problems at the boundaries of a domain: the "surface effect" and the difficulty of imposing the (non-local) boundary conditions. The surface effect occurs due to incomplete neighborhoods near boundaries, causing unrealistic stiffness variations while boundary conditions are often managed with fictitious layers. In addition, non-locality also affects the simulation of a bimaterial interface, which requires the definition of interaction laws between points belonging to different materials. These interactions are confined to a layer whose size is proportional to the horizon value, which represents the maximum distance at which two points interact, leading to a gradual change in the mechanical properties of the layer. Conversely, the peridynamic modelling of a sharp bimaterial interface is still an open problem, despite the various approaches developed [2].

The authors propose an effective method to tackle this issue, inspired by a strategy designed to mitigate the surface effect and impose boundary conditions [3]. The bimaterial interface is modelled assuming, at first, that the two material domains are separate. On the boundaries of the two bodies, which represented the interface and are now free boundaries, layers of fictitious nodes are introduced. The displacement of the fictitious nodes is determined by Taylor series expansion as a function of the displacements of the nearest real nodes, significantly reducing the surface effect. Finally, surface nodes are introduced on the boundaries [3]. These nodes represent the interactions between the internal nodes of a material domain and the fictitious nodes surrounding the body. By imposing equality of displacements between surface nodes, located at the same coordinates but associated with different material domains, it is possible to model a sharp bimaterial interface in a peridynamic model.

The accuracy of the proposed approach is assessed by means of several numerical examples (1D, 2D cases). Simulation results (displacement field) of peridynamic models with bimaterial interfaces, when compared with those obtained from classical continuum mechanics, in the case of uniform strain problems, are in excellent agreement.

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Enhanced Phase-Field Model: Parametrization of Void Inclusion for Material Degradation – CFRAC 2025

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ABSTRACT

The phase-field method has become a powerful computational tool for addressing problems in fracture mechanics. Based on Griffith's criterion [1], phase-field models are grounded in solid physical principles, which gives them reliability and robustness. However, the specific implementations of these models (i.e. the definition of degradation and dissipation functions) often rely on analytical expressions that, while producing accurate results, lack a clear physical interpretation [2][3].

In earlier research, we explored degradation as the homogenization of a microstructure with a void inclusion. This approach offered some initial insights into how it might relate to traditional phase-field models. However, it had limitations because the void was described using a single parameter that mainly represented its size.

In this paper, we extend this methodology by describing the void inclusion with additional parameters that define its shape and orientation within the microstructure. This refinement aims to make the material's degradation behaviour more adequate and adaptive to the macroscopic conditions. Furthermore, the microstructural information may help in determining the path of macroscale fracture with fewer elements, thereby reducing the computational effort typically required by phase-field methods.

The results obtained have been validated using benchmark problems and compared with phase-field models widely used in the community.

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Orthotropic phase field fracture model implementation including several failure mechanisms

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ABSTRACT

The phase field fracture model has attracted the attention of the scientific community due to its ability to capture complex crack patterns with an elegant mathematical foundation. Its extension to anisotropic and orthotropic materials is currently a research topic. An orthotropic phase field model could be applied to study materials that are currently of interest, such as composite materials. With that aim, this work presents an orthotropic phase field fracture model [1] implementation in the commercial finite element code Abaqus. The model allows to discriminate several failure mechanisms, such as fibre failure and transversal failure in unidirectional composite plies. In addition, a Lagrange multiplier approach has been considered to account for damage irreversibility [2]. The proposed model addresses some issues concerning a single damage variable model with a structural tensor [3] and, in general, offers a better crack path prediction in unidirectional composite lamina.

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Adaptive phase-field modeling of fracture propagation in layered media: effects of mechanical property mismatches, layer thickness, and interface strength

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ABSTRACT

Fracture propagation in layered media is studied using an adaptively refined phase-field method. The intricate interplay between cracks and interfaces in layered media is studied through two broad categories of models: (a) perfectly bonded and (b) imperfectly bonded interfaces. The effects of mechanical property mismatches between the middle and extreme layers, middle layer thickness, and confinement pressure on the macroscopic growth are studied through three-layered sandwich models with perfectly bonded layer interfaces. It is observed that while the elastic stiffness mismatch between the middle and extreme layers has little consequence on the eventual crack geometry, the critical energy release rate mismatch significantly influences it. The models fail through a single through-going fracture for low mismatches in critical energy release rates. However, for intermediate and high mismatches, fragmentation of the middle layer is observed. The models with high mismatches also reveal significant delamination along the layer interfaces prior to eventual failure. Additionally, layer thickness and confinement pressure are found to inversely affect the number of fragments in the middle layer and the delamination along the layer interfaces, respectively.

A phase-field method for modeling imperfect interfaces is introduced by supplementing the usual bulk elastic and crack surface energy terms with an interface energy term evaluated as another surface integral at the layer interfaces. The proposed approach is validated through two benchmark examples. The method is subsequently applied to study the combined effects of mechanical property mismatch and interface strength on the macroscopic crack growth through imperfectly bonded layer interface models. It is observed that for relatively strong interfaces (>50% of their original strength), the mechanical property mismatch plays a dominant role in governing the macroscopic crack growth. On the other hand, once the imperfect interface strength is <50% of its original strength, the material primarily fails at the interface. Finally, the robustness of the proposed method is illustrated through a seven-layered model where the mechanical properties of the individual layers, the layer thicknesses, and interfacial strength are all allowed to vary simultaneously. The results of this study provide interesting insights into the influence of mechanical properties, geometric properties, and interface strength on the macroscopic failure mechanisms in layered materials.

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Electromechanical Analysis of Fracture Properties in Conductive Media with Complex Microstructures

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ABSTRACT

The rapid advancement of high-power semiconductor devices, such as wide-bandgap silicon carbide (SiC) and gallium nitride (GaN) devices, has led to demands for power modules with higher power densities and the ability to operate at elevated temperatures. These advancements impose stricter requirements on packaging materials and bonding techniques. In recent years, low-temperature sintering of nanosilver pastes has emerged as a promising lead-free bonding solution for high-frequency and high-power applications. The development of these high-performance conductive materials relies on understanding how their microstructure governs their electro-mechanical performance under mechanical loading. This study presents a numerical framework for analysing the fracture properties of sintered conductive materials with complex microstructures, providing a novel approach to characterizing the interplay between mechanical strains, crack formation, and electrical failure.

This framework uses an electro-mechanical phase-field model to predict resistivity changes caused by crack propagation in the solid microstructure [1]. The analyses are performed on microstructural volume elements (MVEs) generated from synthetic models informed by the composition of raw material and sintering conditions or experimental FIB-SEM images and CT scans. These MVEs enable the derivation of homogenized mechanical and electrical properties, offering insights into the effects of porosity, tortuosity, and ligament length on material performance. To capture the brittle fracture effects typical of these material systems, a modified dissipation-based arc-length solver is employed, ensuring robust and accurate simulations despite snap-back behaviour [2].

The focus of this presentation is on evaluating fracture-related properties, such as microstructural toughness, and their correlation with the degradation of electrical performance. The analysis reveals how microstructural features and control parameters, including metallic particle size distribution and sintering intensity, influence fracture-driven electrical failure.

The framework's capabilities are demonstrated through the analysis of silver sintered joints, a critical application in power packaging. The derived insights link processing parameters to fracture properties and failure mechanisms, enabling the predictive design of conductive materials. By integrating numerical modelling with experimental data, this approach accelerates the development of optimized metallic nanoparticle pastes, fostering improved electro-mechanical performance for applications requiring robust conductive materials.

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An extended phase-field method for the efficient simulation of fracture processes

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ABSTRACT

During the last years, the phase-field method for fracture has gained a lot of attention. It has become the most frequently used method for the simulation of quasi-static and dynamic fracture processes for brittle and ductile materials. Its biggest advantages are the simplicity of the implementation and the fact that it can capture crack propagation, branching, coalescence and initiation without the evaluation of additional criteria in a post-processing step. Despite its great success, the classical phase-field method has one severe disadvantage if standard Lagrange finite elements are employed. Due to the necessity of very fine meshes in the vicinity of an existing crack and its front, the computational effort is very high. This computational effort is further amplified by the highly nonlinear behaviour even for the simulation of linear elastic fracture mechanics processes.

The extended phase-field method (XPFM) combines the phase-field method for fracture with concepts from the extended/generalized finite element method. The concept aims at a significant reduction of computational effort in comparison to the standard phase-field method while keeping the advantages of not having to explicitly track the crack geometry and introduce additional crack propagation criteria.

The XPFM is based on a transformed phase-field ansatz in combination with an enriched displacement field ansatz which depends on the phase-field. In the current approach, the enrichment function of the displacement field is formulated in a discrete way which avoids the potentially difficult calculation of the crack geometry. The enrichment function is calculated by solving phase-field dependent Laplacian equations on element level which can be done in an efficient way.

In this contribution the XPFM, its algorithmic treatment as well as its application to common academic examples is presented.

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Gradient Projection BFGS Monolithic Scheme for Phase-field Crack Simulation: Solver Robustness and Irreversibility Enforcement

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ABSTRACT

A phase-field monolithic scheme based on the gradient projection method is developed to model crack propagation in brittle materials under cyclic loading[1]. As a type of active set method, the gradient projection method is particularly attractive to enforce the irreversibility condition imposed on the phase-field variables as bound constraints, or box constraints. This method has the advantages of allowing the rapid change of active constraints during iterations and computing the projected gradient with a negligible cost. The gradient projection method is further combined with the limited-memory BFGS (L-BFGS) method to overcome the convergence difficulties arising from the non-convex energy functional[2]. A compact representation of the BFGS matrix is adopted as the limited-memory feature to avoid the storage of fully dense matrices, making this method practical for large-scale finite element simulations. By locating the generalized Cauchy point on the piecewise linear path formed by the projected gradient, the active set of box constraints can be determined. The variables in the active set, which are at the boundary of the box constraints, are kept fixed to form a subspace minimization problem. A primal approach and a dual approach are presented to solve this subspace minimization problem for the remaining free variables at the generalized Cauchy point. Several 2D and 3D numerical examples are provided to demonstrate the robustness of the solver and the effective enforcement of the irreversibility condition. The proposed method is further compared with two other phase-field solving techniques regarding the convergence behavior. To ensure a fair comparison, the same problem settings and implementation techniques are adopted. The proposed monolithic scheme provides a unified framework to overcome the numerical difficulties associated with the non-convex energy functional, effectively enforce the phase-field irreversibility to ensure the thermodynamic consistency, and alleviate the heavy computational cost through adaptive mesh refinement in 2D and 3D phase-field crack simulations.

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How to introduce sharps cracks in continuous damage models using the eXtreme Mesh deformation approach (X-Mesh) : a 1D study

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Continuous damage models are widely used to model the propagation of cracks, since they can handle complex cracking processes, from nucleation to coalescence and branching. However, these approaches do not explicitely model cracks opening, which is necessary to avoid numerical issues when the damage variable d tends to 1, or to model contact phenomenon between cracks lips for instance. In this work, we will see how to use the eXtreme Mesh deformation approach (X-Mesh) introduced in [1] to insert macro-cracks opening inside a continuous damage model. In particular, we will consider two continuous approaches to fracture: the Phase-field approach [2] which has been widely used to model the failure of material since the last few years, and a more recent one, the Lip-field approach [3]. Both formulate the mechanical problem to be solved as the minimization problem of an incremental potential, and introduce a characteristic length parameter ℓ_c to avoid mesh dependency, the main difference being how this parameter ℓ_c is taken into account.

The main idea of X-Mesh as it is presented in [1] is to move the nodes of a finite element mesh to have a time continuous, sharp representation of a moving front (for instance in [1], a phase-change front). These nodes movements allow to model topological changes of the front, including coalescence and splitting. Note that only the position of the mesh element nodes changes, the topology of the mesh being fixed (that is, the connectivity between the nodes), which is much cheaper that full remeshing. For fronts where only the derivative of the quantity of interest if discontinuous, having only a line/surface of nodes in 2D/3D on the front is enough; however, in the case of cracks where the displacement field is discontinuous, the key idea will be to move nodes to create zero measure elements at the cracks location.

Since both Phase-Field and Lip-field formulate the mechanical problem to be solved as an optimisation problem, where the unknown are the displacement and damage fields, it is natural in the X-Mesh framework to consider the mesh nodes position as an additional unknown. In this work, we will show on 1D examples that by optimising the mesh nodes position, zero measure elements appear when the damage variable tends to 1, allowing jumps of the displacement solution. We will compare the results obtained by this approach to results obtained with X-Mesh, focusing on the solution behavior when $d \to 1$.

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Understanding Sources of Errors and Dissipation in Phase Field Implementation for Achieving Trustable Simulations

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ABSTRACT

The phase field method has become a popular technique in the field of computational solid mechanics. This might be attributed to a number of factors. For example, the phase field method offers an elegant way to modeling and predicting complex fracture propagation, including branching and merging. One of the primary benefits of the phase field approach is that it does not require prior knowledge of the fracture path, hence eliminating the necessity of mesh treatment methods and crack tracking algorithms.

Nevertheless, the method has some limitations and disadvantages, such as the computational cost, as a fine mesh is needed near the crack surface to achieve smooth smear out of discontinuity. Additionally, the result depends on several components such as but not limited to the degradation function, and the regularization length. In addition, the stress and displacement fields close to the crack tip become more diffuse due to the smearing of the crack interface. Furthermore, the method's coupled nonlinear system of equations poses a number of challenges for numerical solvers, particularly when it comes to enforcing physical constraints like irreversibility and compressive stress isolation. Achieving trustable simulations requires a good understanding of the physical meaning of each parameter, which is often challenging. As a consequence, many phase field simulations are merely numerical exercises that cannot be relied on for engineering design.

To overcome these limitations, it's critical to use the phase field method according to the best practices, which requires an understanding of the source of error when describing a discontinuity by phase field, and the influence of each component, including the regularization length, degradation function, mesh size, solving scheme, etc. Incompatibility of these parameters may result in a significant difference between the phase field solution and the solutions obtained through discrete modeling approaches.

The aim of this work is to move towards more trustable simulations by determining the factors that set the gap between discontinuous solutions and phase field solutions. We seek to determine the best techniques and guidelines, in order to obtain significant results with the phase field. First, we focus on crack description using the phase field. We discuss the techniques used to describe pre-existing cracks and provide analytical estimates for the regularization and discretization errors. Next, we examine the crack propagation regime and dissipation by comparing it with LEFM solutions, and highlight the discrepancies and their causes. Last, we go into the strategies that can be employed in order to overcome the discrepancies and guarantee a trustable and meaningful result when using the phase field method.

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A quantitative comparision of different phase-field damage formulations, through a fully explicit time integration resolution.

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Abstract

Transient damage evolution and fracture propagation present significant challenges in numerical modeling, stemming from both poorly understood phenomena and inherent numerical model difficulties. Several strategies have been developped to better understand dynamic crack propagation, particularly fast transient scenarios. Among these, gradient damage modeling considering a damage phase-field evolution has gained popularity and has known significant advances. This approach has successfully reproduced key phenomena such as nucleation, branching, and kinking. However validation of this numerical model with benchmark experiments in transient regime remains a challenging task.

The phase-field damage approach is based on a minimization of a total energy functional and draws its origins from two different approachs : the variational extension of the Griffith's theory proposed by Bourdin et al.[1], and the thermodynamical framework from the Generalized Standard Materials. While the former one does not explicitly extend to dynamic fracture evolution, the latter provides a generic framework for modeling dynamic damage evolution. This model is composed of a coupled system of two equations governing the displacement and the damage evolution. In the dynamic regime, an elasto-dynamic equation is used for the mechanical problem while the damage evolution is modeled through an elliptic [2], a parabolic [3] or a hyperbolic [4] formulation.
This work presents a quantitative comparison of these formulations, using different resolution strategies. While the elliptic damage formulation is solved with an implicit iterative method, the system of equations involving dynamic damage evolution is addressed with a fully explicit time integration. Firstly, the resolution performance of a fully explicit time integration has been assessed, particularly focusing on the stability conditions of the integration scheme. Secondly, the ability of the three different damage formulations to reproduce transient damage evolution has been evaluated numerically. The phase-field approach with dynamic damage evolution has shown promising capabilities in reproducing transient damage phenomena. However, the hyperbolic formulation, in particular, can exhibit over-damaged regions or inconsistencies in enforcing the damage irreversibility condition during simulations.

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Improving the Cost of Phase-Field Fracture Computations - Making 3D Crack Propagation Simulations Viable

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ABSTRACT

The phase-field approach to fracture modeling has emerged as an attractive alternative to the conventional sharp crack modeling approaches such as XFEM; see for instance [1] and the references therein. Primary reasons for such heightened attention include suitability to be implemented in a standard confirming finite element framework and the promise for the development of a unified framework capable of dealing with both existing cracks as well as the nucleation of new ones. The diffuse approximation of a sharp crack, however, necessitates the usage of extremely fine finite element meshes in order to adequately resolve the diffuse crack zone. Furthermore, sufficiently small load increments are required, even more so in case of large strain problems, for accurate description of the fracture process. Moreover, adopting a two-way coupled staggered approach to solve a load-step results in several such staggered iterations, especially during the brutal crack propagation regime, thereby further aggravating the computational complexity of the numerical algorithm. Consequently, despite the rapid development of the phase-field fracture models in the last two decades, simulation of crack propagation in complex geometries, especially in three-dimensions, still remains a challenge [2]. In this work, we describe two improvements for reducing the computational cost of a phase-field fracture simulation. The first one being exploring efficient iterative linear solvers and preconditioners since the solution of the displacement linear system arising during each Newton iteration within the staggered scheme accounts for majority of the required compute time. Secondly, an alternative stopping criterion based on the change in total energy of the system is proposed for the staggered iterations. Numerical examples with increasing computational complexity are presented to highlight the improvement in computational cost obtained by the aforementioned optimizations.

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The Lip-field approach for fracture: state of the art

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ABSTRACT

The Lip-field approach is a regularization method for softening material models. It was applied to damage and softening (visco)-plasticity models both in 1D and 2D scenarii.

The incremental potential used in the Lip-field approach is the nonregularized one. The regularization comes from the addition of a Lipschitz constraint on the damage field (or adequate (visco)-plastic quantities). In other words, the free energy does not depend on the damage gradient. The search of the displacement and damage fields from one time-step to the next is based on an iterative staggered scheme. The displacement field is sought for a given damage field. Then, a Lipschitz continuous damage field is sought for a given displacement field. Both problems are convex. The solution to the latter benefits from bounds proven in [1]. The implementation of the Lipschitz regularity constraint on a finite element mesh and details of the overall solution scheme will be presented. Numerical examples will demonstrate the capability of the approach [2]. The relationship between the phase-field and lip-field approaches will also be discussed.

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Influence of history variable on phase field damage prediction

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ABSTRACT

Predicting the maximum load that a (quasi-)brittle specimen can sustain, along with determining the correct crack path, is a crucial scientific and practical challenge. Over the last few decades, numerous models have demonstrated their ability to predict both critical loads and crack paths effectively. Some of these models include the Thick Level Set (TLS) models [9, 10], Phase Field damage models [3, 7], Peridynamics [5, 6], and more recently, the Lip Field damage [4, 8].

The Phase Field damage model has been widely adopted over the past few decades, primarily building on the foundational work of Bourdin et al. [2]. Enthusiasm within the mechanics community surged following the influential publication by Miehe and co-workers [7]. In particular, the introduction of a history variable simplified model implementation and facilitated the incorporation of irreversibility conditions.

In this work, we present a comparison between damage results obtained from the Phase Field damage model when a history variable is used and when it is not. Several numerical tests are conducted to illustrate the differences between the two approaches. Finally, we simulate selected experimental tests using both formulations of the Phase Field damage model to further demonstrate their respective strengths and limitations.

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Application of the gradient-enhanced damage model based on Hamilton principle solved by neighbored element method

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ABSTRACT

Traditional damage models make it difficult to accurately and efficiently simulate large 3D models They usual deal with an increased number of nodal unknowns, which remarkably increases the computation cost due to the convergent problem. We thus adopt a neighbored element method to solve the gradient-enhanced damage model based on Hamilton principle [1]. It combines the finite element method and generalized finite difference method to optimize the convergent problem during the simulation, which can significantly decrease the computation time maximum to one or two magnitudes. It has already been applied to solve the specified problem such as damage in artery when a stent is placed or the damage during forging and the quenching process.

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A phase-field model for the brittle fracture of Euler-Bernoulli beams

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ABSTRACT

Damage gradient models seek to simulate fracture mechanics by modulating the material stiffness. Within this framework, a singular scalar field representing damage is commonly utilized to globally decrease elastic energy. However, when considering structural models like beams and plates, this approach often fails to adequately capture important aspects due to the interaction between stretching and bending contributions.
We propose a model for planar Euler–Bernoulli beams that incorporates the following features: firstly, we utilize two phase-field damage parameters to describe material damaging, specifically addressing the 'erosion' occurring above and below the original, undamaged beam; secondly, we assume a simple linear dependence of the axial stress field on the thickness coordinate, along with linear dependence on the axial force and bending moment. By appropriately identifying the constitutive response, our model effectively considers the coupling between stretching and bending induced during through-the-thickness damage, demonstrating good agreement with 2D observations.

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Modeling and Simulation of Incompatible Deformations in Solids with dislocation microstructure : A Strain-Gradient Approach with Finite Element Implementation

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ABSTRACT

This work deals with the macroscopic modeling of solid continua, typically single crystals, undergoing incompatible deformations due to the presence of microscopic defects like dislocations. We propose a novel approach relying on a geometrical description of the medium by the strain tensor and the representation of internal efforts using zero-th and second-order strain gradients in an infinitesimal framework. The novel kinematic variable is the strain incompatibility, a second-order tensor involving second derivatives of the strain itself. At the same time, energetic arguments allow to monitor the corresponding tangent moduli. We provide mathematical and numerical results to support these ideas in the framework of isotropic constitutive laws. Discretization is made by means of Finite elements. The numerical method is innovative, based on concepts of exterior calculus and the notion of "Complexes", here applied to the so-called elasticity complex. New elements are implemented to address the specific tensor and 4th-order nature of the equations. We will present the model and a series of numerical simulations on several benchmarks examples in plasticity. Hencky perfect plasticity as well as time-incremental plasticity with hardening will be presented. Comparison with classical models will be provided, in order to assess the validity of our model and highlight its main features. Comparison of the classical and new FE results will be presented as well. This is a joint work with Nicolas Van Goethem (Lisbon), Samuel Amstutz (Avignon), Thien-Nga Lê (École polytechnique de Palaiseau) and Francis Aznaran (Notre Dame University).

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Dynamic fragmentation with the cohesive Lipschitz (CLIP) approach

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The dynamic fragmentation of materials under extreme loading conditions, such as explosions and high-velocity impacts, poses significant challenges in predicting and understanding fragment behavior, particularly in aerospace and space debris management applications. To address these challenges, the Cohesive LIPschitz (CLIP) model is proposed as a novel theoretical framework for fracture. The CLIP model combines the strengths of both cohesive and diffuse crack models, aiming to overcome key limitations in dynamic fragmentation simulations, such as mesh dependency and high computational costs while maintaining high accuracy in predicting fragment behavior.

The CLIP model is inspired by two established fracture modeling approaches: the Cohesive Zone Model (CZM) [1] [2] and the Lip-field (LIP) approach [3] [4]. The CZM provides an explicit representation of crack surfaces, making it effective for modeling fragment interactions and contact mechanics. However, it suffers from mesh dependency, where the underlying mesh significantly influences crack paths and fragment shapes. On the other hand, the LIP model, a diffuse crack approach, eliminates mesh dependency by distributing damage across a finite region. While this ensures robust and mesh-independent results, it increases computational demands and complicates the identification of individual fragments. The CLIP model combines these complementary approaches, achieving a balance between robust crack representation and reduced sensitivity to mesh configurations.

The CLIP model employs a variational formulation of fracture mechanics, which evolves the displacement field u and damage field d over time by minimizing an incremental potential. This formulation creates cracks in a cohesive manner, explicitly representing crack surfaces while inducing a diffuse damage zone around them. The cohesive and diffuse damage fields are linked through a Lipschitz-type relation, ensuring a smooth transition between localized and distributed damage. The CLIP model also replicates the behavior of a linear CZM, providing a familiar yet enhanced framework for fracture modeling. This hybrid approach ensures accurate fracture representation while addressing mesh dependency challenges.

The results from 1D quasi-static and explicit dynamic analyses will be presented, demonstrating the model's ability to capture fracture behavior in simplified scenarios. Preliminary findings from ongoing 2D explicit dynamic simulations will also be shared, highlighting the CLIP model's potential to address more complex fracture scenarios and contribute to advancements in dynamic fragmentation modeling.

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Efficient high-cycle fatigue predictions by means of numerical simulations

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ABSTRACT

High computational costs frequently limit the practicality of fatigue simulations for complicated structures or long-term predictions. This work describes a novel and fast methodology for modeling fatigue that avoids the lengthy processing periods required for cycle-by-cycle simulations. The introduction of a coordinate transformation from the time parameter to the cycle number results in a novel model with significant decrease in computational expenses. Our method enables the efficient development of force-displacement curves, as well as the study of low- and high-cycle fatigue and the endurance limit. The strategy, based on the Hamilton principle of stationary action [1] and implemented using the Neighbored Element Method [2], is demonstrated to be robust and effective in a variety of boundary value problems. The experimental validation is shown and based on the result of a single fatigue test while predicting various stress amplitudes.

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Phase-field modeling of high-cycle fatigue behavior in L-DED 18Ni-300 maraging steel components

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ABSTRACT

Laser-based directed energy deposition (L-DED) has emerged as a transformative additive manufacturing technology, enabling layer-by-layer fabrication of complex metal component, meeting demands of various industrial sectors, particularly aerospace and automotive. However, concerns about mechanical performance and fatigue behavior of these parts have limited its broader industrial adoption. These limitations primarily originate from inherent manufacturing defects such as porosity, inclusions, and surface anomalies that can compromise structural integrity and fatigue properties. Since its emergence, phase field method (PFM) in fracture has been used in wide range of material settings, including additively manufactured components, notably in [1-3].

The fatigue behavior of structures using PFM framework has been developed and investigated in recent years [4,5]. In this work, we implement an efficient phase field framework to investigate the behavior of high-cycle fatigue (HCF) cracks with particular interest in cyclic crack advances in components produced using L-DED. The framework incorporates mean load effects on fatigue history variable. To accelerate HCF simulations, we implement a staggered solution method based on a modified Newton-Raphson strategy which reuses factorized tangent stiffness matrices across multiple loading cycles. To further optimize computational efficiency, we develop an adaptive switching scheme between full and modified Newton-Raphson methods, where tangent stiffness updates are dynamically controlled based on solution stability indicators. Through parametric studies, we evaluate the model's performance in terms of computational efficiency and prediction regarding the evolution of complex crack topologies under cyclic loading. Furthermore, the framework is successfully validated against the experimental crack growth rate diagrams and captures the orientation-dependent fatigue behavior, where specimens with cracks propagating across deposited layers exhibit longer fatigue life compared to specimens where cracks grow parallel to the layer interfaces.

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A pseudo-dynamic phase-field framework for brittle fracture

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ABSTRACT

The enforcement of global energy conservation in phase-field fracture simulations has been an open problem for the last 25 years. Early on, it was observed that the occurrence of unstable fracture is accompanied by a loss in the total potential energy, which in turn violates the law of energy conservation. Unstable fracture is characterized by rapid crack growth and can occur even in cases that involve purely quasi-static, displacement-type loading. In the latter, it can be understood as the occurrence of finite crack growth for an infinitesimal increase in load. This is often seen in crack nucleation events but can also occur in other instances. Early attempts at enforcing energy conservation took the form of backtracking schemes, which are based on a global minimization paradigm.

Recently, it has been more understood that unstable fracture is an inherently dynamic phenomenon and thus cannot be adequately resolved within a purely quasi-static framework. Nevertheless, it is not clear whether the issue can be addressed simply by switching to a fully dynamic framework, since this introduces additional problems, such are stricter requirements on mesh refinement and the need to properly model damping as well as energy dissipation at boundaries. Equally important is how crack regularization affects the propagation of stress waves in comparison with sharp cracks, which has not been adequately studied.

In this talk, we present an alternative paradigm: a pseudo-dynamic framework that aims to recover energy conservation without resorting to global minimization. Instead, we adopt a heuristic approach to include such dynamic effects within an otherwise quasi-static framework. This enables us to avoid having to solve the full dynamic linear momentum equation, while still retaining the flexibility to simulate crack evolution anywhere within the spectrum defined by full energy conservation at one end, and maximal energy loss at the other. Using data from recently published experiments, we demonstrate that with the proposed framework, we can closely match experimental load-displacement curves in a way that is impossible using classical phase-field models.

A Time-homogenization Scheme for Brittle and Ductile Fatigue Simulation with the Phase Field

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ABSTRACT

The fatigue fracture brings severe mechanical failures. In recent years, the phase field approach for frac-ture has been extended to fatigue fracture. In this study, we propose an efficient acceleration scheme for the phase field approach based on a concurrent time-scale homogenization theory. In this scheme, the fatigue fracture problem is decomposed into a macrochronological problem and a microchronological problem, and is accelerated with the macrochronological time steps adaptively determined. Throughout the whole simulation, the macrochronological time step is monitored, and is corrected by a predictor-corrector strategy if necessary. This scheme is able to accelerate fatigue fracture simulations without sacrificing much accuracy, and can be up to 200 times faster than direct numerical simulations in some cases. For certain force-controlled examples, the proposed scheme, equipped with the arc-length control, is able to reproduce Paris' law with a correlation coefficient higher than 0.91 in the logarithmic scale. For more details, see [1].

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Minisymposium TF:

Theory of fracture, crack propagation criteria and crack tracking algorithms

Organized by A. Pandolfi and M. Ortiz

The Brazilian Fracture Test Explained, with Application to 3D Printed Mortar

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ABSTRACT

Since its introduction in the 1940s [1] until present times, the so-called Brazilian test has been embraced by practitioners worldwide as a method of choice to indirectly measure the tensile strength of concrete, rocks, and other materials with a large compressive strength relative to their tensile strength. This is because of the ease that the test affords in both the preparation of the specimen (a circular disk) and the application of the loads (two platens compressing the specimen between them). Yet, this practical advantage has to be tempered by the fact that the observations from a Brazilian test — being an indirect experiment in the sense that it involves not uniform uniaxial tension but non-uniform triaxial stress states throughout the specimen — have to be appropriately interpreted to be useful. In this talk, I will present a complete quantitative analysis of where and when fracture nucleates and propagates in a Brazilian test and thereby establish how to appropriately interpret its results [2]. I will do so by making use of the phase-field fracture theory introduced in [3,4], which has been recently established as a complete theory of fracture nucleation and propagation in elastic brittle materials. After the general analysis, I will present simulations and experiments for a newly 3D printed mortar, as well as a new protocol to deduce the tensile strength of a material from a Brazilian test that improves on the current ISRM and ASTM standards. I will close with some general remarks about how critical it is to accurately account for the entire strength surface of materials in order to be able to describe fracture nucleation in boundary-value problems where the stress fields are highly non-uniform.

This work was done in collaboration with S. Saha, Y. Liu, A. Kumar, J.R. Roesler, and J.E. Dolbow.

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Cracquelure in paintings under moisture variations

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ABSTRACT

Craquelure poses a substantial threat to both the aesthetic and material integrity of artworks [1],[2]. To address this, a multi-physics numerical model has been developed to simulate the hygro- mechanical behaviour of multilayered paint system exposed to varying levels of relative humidity. The model captures interactions among the key layers—canvas, glue, and paint—while integrating the humidity-dependent changes in material properties, including elasticity, tensile strength, and moisture expansion, to accurately represent the mechanical response of paintings. By coupling moisture diffusion with stress analysis, the model predicts the initiation and propagation of cracks caused by humidity-induced stresses through a phase-field approach to fracture. Rupture mechanisms are governed by an energetic competition between fracture in the paint layer or delamination at the interface.

Validation tests confirm the model's ability to replicate rupture mechanisms characteristic of craquelure. Additionally, the model has been applied to representative scenarios, providing valuable insights into moisture-driven craquelure patterns. This tool offers significant potential for the development of preventive conservation strategies, contributing to the long-term preservation of cultural heritage artworks

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Influence of viscosity on crack propagation in elastomers

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ABSTRACT

Fracture experiments on pre-stretched elastomeric membranes, as reported in [1,2], demonstrate that viscosity significantly influences crack propagation speed. Specifically, a rapid increase in crack velocity is observed, attributed to the abrupt transition of the material state from rubbery to glassy ahead of the crack tip.

This paper introduces a variational model for crack propagation in elastomers, utilizing a phase-field fracture approach. The model incorporates both a viscous macro-stress, representing the strain rate dependency, and a viscous micro-stress, capturing rate-dependent micromechanical phenomena involved in the fracture process.

The proposed model is implemented in a FEM code, and numerical simulations are conducted to analyse the impact of the rubbery-to-glassy viscous transition on crack propagation speed.

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Fracture of soft composites: modeling and experiments

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ABSTRACT

We present theory and simulations of fracture of soft staggered composites [1] based on the generalization and finite element implementation of the material sink approach [2]. Results of the simulations are compared to experiments with 3D-printed soft composites [3,4]. In addition, the experiments allow an assessment of the stress-based versus energy-based failure criteria [5]. Results of the assessment are intriguing.

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Variationally Consistent Virtual Element Modeling of Mixed-Mode Cohesive Crack Propagation

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ABSTRACT

The Virtual Element Method (VEM) [1], an extension of the finite element method allowing for the use of polygonal and polyhedral elements with arbitrary number of nodes, is known for being almost completely insensitive to element distortions. Exploiting this appealing feature and based on a recently presented variational formulation of linear elastic self-stabilized Virtual Elements (VEs) [2], we propose a strategy for the simulation of mixed-mode cohesive crack propagation in a mesh of originally self-stabilized Virtual Elements (VEs).

As in other works (see, e.g. [3-4]), the propagating cohesive crack is accommodated within existing first-order quadrilateral VEs by simply adding new edges separated by a cohesive interface. The new mixed variational framework, incorporating the crack fracture energy, allows for a higher order, independent modeling of stresses at the tip of the cohesive process zone and, hence, for a more accurate assessment of crack propagation conditions and direction.

Though the quadrilateral VEs are initially stable, the added edges make the obtained VEs unstable and a new procedure for the stabilization of the VEs crossed by the crack is developed. The cohesive crack is allowed to propagate when the maximum principal stress at the fictitious crack tip exceeds the cohesive strength. A stress smoothing procedure, taking advantage of the higher order stress model, is adopted to improve the quality of the local stress evaluation. The crack propagation then occurs in a direction perpendicular to the direction of the maximum principal stress.

The proposed method is successfully validated by application to several benchmark problems.

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Efficient Calculation of the Energy Release at Eigenfracture

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ABSTRACT

Regularised formulations of the variational free-discontinuity problem have been shown to yield powerful computational methods towards fracture from brittle elasticity to inelastic multi-physics and multi-scale problems. To overcome the presence of the crack domain Γ at the integral bounds in

$$E(u,\Gamma)=\int_{\Omega/\Gamma}\psi(Du)\,dV+G_c\int_{\Gamma}dA\rightarrow Min,$$

the fracture energy is evaluated through a volume integral on the introduced crack area density function $\gamma_l(p)$ in phase-field fracture or through the crack neighbourhood volume $\Omega_\Gamma(l)$ in eigenfracture [1]. Furthermore, the potential energy ψ is evaluated on that portion $D^a u$ of the distributed derivative Du, which represents the bulk material deformation and neglects any contribution from the crack deformation, leading to

$$E(u,\Gamma)=\int_{\Omega}\psi(D^a u)\,dV+\frac{G_c}{2l}\int_{\Omega_\Gamma(l)}dV\rightarrow Min.$$

By applying the space of *special functions of bounded variation (SBV)* [2] to the brittle fracture problem, the decomposition $Du=D^a u+D^j u$ was shown to exist uniquely.

This contribution presents the framework of Representative Crack Elements (RCE) as a general solution scheme to solve this decomposition and, serving as a substitute for artificial energy split models in phase-field fracture and eigenfracture [3]. The benefits of the method are demonstrated through illustrative examples for inelasticity, finite deformations, crack surface friction, multi-physics, as well as the faster Γ-convergence.

Finally, the approximative calculation of the energy release in eigenerosion [4] is investigated and the missing mesh convergence is elaborated. An efficient method to address and resolve this approximation is proposed and analysed.

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Crack propagation criteria with bond-associated peridynamics

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Peridynamics is a nonlocal continuum mechanics formulation known for its ability to model damage and fracture phenomena. However, many peridynamic formulations have significant discretization errors in elastic modeling due to nonlocality and surface effects. There are several approaches to mitigate these limitations, such as the correspondence formulation, which utilizes an approximated deformation gradient to calculate stress forces. Although this reformulation improves the accuracy of elastic modeling, it introduces instabilities. The bond-associated peridynamic formulation is a promising solution, as it combines the advantages of bond-based for modeling fracture and the accuracy of the correspondence formulation for elastic modeling without instabilities. In standard peridynamics formulations, crack propagation is mostly modeled with a critical bond strain criterion. With bond-associated modeling, this can be reconsidered, as stress tensors are calculated for each bond, making it possible to introduce new criteria. This study presents a comprehensive review of crack propagation criteria especially for bond-associated peridynamics. Explanatory examples and intersting simulations are provided, showcasing the capabilities and practical relevance.

Keywords:
Peridynamics, crack propagation, fracture criteria, bond-associated peridynamics

Arc-length methods for the modeling of rate-independent fracture

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ABSTRACT

The computational modeling of rate-independent quasi-brittle fracture continues to pose a scientifical challenge - for example, due to unstable or brutal crack growth. In engineering science, arc-length techniques have proven to be particularly effective for such phenomena. Alternatively and with the mathematical community in mind, so-called balanced viscosity solutions are often considered. As shown, e.g., in [1], they can also be interpreted as arc-length methods. In this talk, the physical principles underlying arc-length methods and their connection to balanced viscosity solutions will be explored. Numerical experiments are presented to illustrate the stability and efficiency of these methods and to demonstrate their potential for the accurate simulation of rate-independent systems.

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A robust and efficient method for crack features extraction from field data

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ABSTRACT

The displacement field on a neighbourhood of a crack tip is described accurately within the Linear Elastic Fracture Mechanics framework by Williams Eigenfunction Expansion Form (EEF) [1]. The parameters of these series are referred to as Williams coefficients and have various physical meanings. For example, they may be used to compute important quantities of interest in fracture mechanics such as the stress intensity factor K (order $n = 1$) or the T- and B-stresses ($n = 2$ and $n = 3$ respectively).

Various approaches exist to determine K from a measured displacement field, for instance from the J- or interaction integrals. Nevertheless, they cannot be used to estimate subsingular terms ($n \geq 2$). Another common method, which consists in projecting the displacement field onto Williams EEF with the L^2-norm, strongly depends on the projection domain and is thus very inaccurate. For these reasons, we investigated an alternative approach based on Bueckner conjugate work integral [2] for the determination of Williams coefficients. As demonstrated by Chen [3], this integral is path-independent and provides a scalar product in which the terms of the Williams series form an orthogonal basis. More recently, Melching *et al* [4] used these interesting properties to retrieve subsingular terms of the EEF.

We conducted a numerical study to ensure the convergence of Bueckner's contour integral and rewrote it as an Equivalent Domain Integral (EDI). The simulations performed on a test case demonstrate a better accuracy and a higher convergence order of Bueckner's integral compared to the J-integral both for line and volume integration. With one order of convergence higher than J, Bueckner's integral is also more efficient and can be evaluated on smaller integration domains. This is a major breakthrough when dealing with curved cracks, since the evaluation of Williams EEF in the vicinity of the crack is therefore far more robust.

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Towards Pure Griffith Crack Propagation

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ABSTRACT

Variational formulations of Griffith fracture based on global minimization, and even local minimization, intertwine propagation and nucleation. Having the view that Griffith energy competition is a principle only for propagation, we seek a Griffith variational formulation producing only propagation. Starting with the local stability condition in [1], which overcomes several difficulties present with global minimization, we describe corresponding formulations for crack propagation based only on local energy competition between elastic and surface energies, even in the presence of applied loads.

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Fast Fracture in Brittle and Quazi-Brittle Materials – CFRAC 2025

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ABSTRACT

A nonlocal model for fast fracture is introduced consisting of two phases, one elastic and the other inelastic. Evolution from the elastic to the inelastic phase depends on material strength. Existence and uniqueness of the displacement-failure set pair follow from an initial value problem describing the evolution. The displacement-failure pair satisfies energy balance. The length of nonlocality ε is taken to be small relative to the domain. The strain is formulated as a difference quotient of the displacement in the nonlocal model. The two point force is expressed in terms of a weighted difference quotient. This evolution provides an energy balance between external energy, elastic energy, and damage energy including fracture energy. For any prescribed loading the deformation energy resulting in material failure over a region R is uniformly bounded as $\varepsilon \to 0$. For fixed ε, the failure energy is discovered to be is nonzero for $d - 1$ dimensional regions R associated with flat crack surfaces. Calculation shows, this failure energy is the Griffith fracture energy given by the energy release rate multiplied by area for dimension = 3 (or length for dimension = 2). The nonlocal field theory is shown to recover a solution of Naiver's equation outside a propagating flat traction free crack in the limit of vanishing spatial nonlocality. The theory and simulations presented here corroborate the recent experi- mental findings of (Rozen-Levy et al. in Phys. Rev. Lett. 125(17):175501, 2020) that cracks follow the location of maximum energy dissipation inside the intact material. Simulations show fracture evolution through the generation of a traction free internal boundary seen as a wake left behind a moving strain concentration.

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Simulating seismic events triggered by fluid injection using a combined cohesive and frictional modelling approach

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ABSTRACT

We employ a porous-mechanical material model with parallel planar microstructures to simulate an in situ induced seismicity experiment conducted on a natural fault [1]. The experiment involves localized fluid injection with a prescribed flux history, which triggers a two-phase slip event: an initial aseismic motion followed by a seismic event marked by a rapid increase in sliding. The porous brittle damage model with cohesive-frictional interfaces [2] is used to describe the fault and surrounding rock behaviour. The goal is to predict the primary observations of the experiment, specifically the activation of macro-fault slipping through a 3D finite element approach combined with a micromechanical brittle damage model. The fault is modelled as a damaged rock segment, containing a network of parallel micro-faults, which helps capture the complex interactions between the fault and surrounding rock, offering a better understanding of the mechanisms driving induced seismicity. By accurately modelling the fault behaviour under fluid injection, this study provides insights into the risks associated with activities such as geothermal energy production, hydraulic fracturing, and CO2 sequestration. The results can inform strategies to minimize potential hazards and enhance the safety and sustainability of these operations.

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Variational mesh adaptation for crack growth

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Moving nodes of a finite element mesh for modeling crack growth has a two-fold interest. On the one hand, we can sharply represent the crack path and its evolution. On the other hand, and more generally, the obtained displacement field can be optimized with respect to energy norm by modifying the reference mesh. We propose an approach that relies on both aspects.

Our starting point is minimizing the energy functional by jointly tuning nodal values and node positions. Observing variations of potential energy with respect to non-material points (*i.e.* nodes) let configurational mechanics come into play. Using the configurational framework to enhance the fracture mechanics mesh is a known approach [1]. But discretizations that have reached configurational equilibrium are often sidestepped due to possible extreme mesh deformations. Thanks to T-FEM method [2], we can now freely perform variational mesh adaptation to obtain null configurational forces on nodes. Obtaining this optimal mesh can be done using several non-convex optimization methods (gradient descent, BFGS, Nesterov's accelerated gradient, *etc.*).

Once this is achieved, the evaluation of Griffith's criterion in brittle material is simplified and, therefore, it enhances the resulting crack growth. Indeed, one can show that an optimal mesh restores the path-independency of Rice's integral. Then, the energy release rate is now sharply approximated by the configurational force at the crack tip. By adding a dissipation term, it becomes possible to finally model crack growth by modifying the geometry itself with possible node nucleations.

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On the Effects of Material Strength in Dynamic Fracture:

A Phase-Field Study

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ABSTRACT

Over the past seven years, full-field analyses of a wide range of classical as well as modern quasi-static fracture experiments on nominally elastic brittle materials have repeatedly identified the material strength surface as one of the key material properties that governs not only the nucleation of cracks, but also their propagation. Central to these analyses are the results generated by the Griffith phase-field fracture theory with material strength introduced in [1,2]. The theory accounts for an arbitrary material strength surface through an external driving force in the evolution equation for the phase-field. In this talk, we extend this model through the addition of inertial forces [3]. The dynamic version of the model is then validated against a broad range of benchmark experiments for dynamic brittle fracture, including the experiments by Kalthoff and Winkler, the Brazilian fracture test, and a recent experiment investigating crack initiation, propagation and branching in soda-lime glass specimens [4]. As expected from the analyses of quasi-static experiments, the simulations make it clear that accounting for the material strength surface as an independent macroscopic property remains essential to explaining and describing experimental observations when inertia is not negligible. This key insight is further illustrated by means of comparisons with results from classical phase-field models, which, by construction, are unable to account for a strength surface that is independent of the elasticity and toughness of the material.

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On the Consistency of Strength-based Nucleation and Griffith Propagation in Phase-field Approximations to Quasi-static Fracture

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ABSTRACT

We examine recent models, [1], [2], [3], [4] etc., that take into account strength-based nucleation and Griffith propagation by way of a so-called *driving force*. We demonstrate that at sufficiently small length scales current phase-field models do not approximate sharp models that allow for unbounded stresses, which are known to occur near crack tips as a consequence of linear elasticity. We introduce a new criterion that regulates exactly when fracture nucleation must occur. With this requirement, we describe modifications that allow for an arbitrary strength surface while being consistent with unbounded stresses in the limit as the length scale approaches zero.

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Preconditioning strategies for solving monolithic phase-field models of brittle fracture

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ABSTRACT

The phase-field approach has emerged as a powerful framework for modeling complex fracture phenomena, such as crack initiation, propagation, branching, and merging. However, solving the resulting nonlinear systems poses significant challenges due to the non-convexity, non- smoothness, and high computational cost associated with the energy functional. To address these issues, we explore nonlinear preconditioning strategies that enhance solver robustness and efficiency.

Our focus includes the development and analysis of advanced preconditioning techniques, such as field-split-based additive and multiplicative Schwarz preconditioners integrated within Newton's method. These strategies exploit the structure of the coupled displacement and phase-field equations to improve convergence rates and solution stability.

Through numerical benchmarks and comparative studies against traditional methods like alter- nate minimization, we demonstrate the efficacy of the proposed strategies in tackling challenging phase-field fracture problems. The results highlight the potential of nonlinear preconditioning to significantly reduce computational costs while maintaining accuracy in modeling intricate fracture processes.

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Following the equilibrium path during crack propagation under quasi-static loads: linear elastic fracture mechanics and phase-field approaches

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ABSTRACT

The equilibrium path [1] of an elastic body with an initial crack represents the sequence of states (displacement and crack geometry) at which crack propagation threshold is met under a specific quasi-static proportional loading sequence. Constructing this equilibrium path requires adjusting the load amplitude to maintain the crack at its propagation threshold throughout its progression. Following the equilibrium path gives the stable and incremental crack propagation, at the cost of neglecting dynamic effects arising during instabilities. Following the equilibrium path in numerical simulations (e.g., phase-field fracture models) ensures controlled and incremental crack propagation so that each crack increment minimizes the energy (in contrast to minimizing the energy over the entire crack path).

This work proposes methodologies to determine the equilibrium path with the frameworks of Linear Elastic Fracture Mechanics (LEFM) and phase-field fracture models. It focuses on the case of a single controlled load, but extensions to more complex loads will also be discussed.

We first examine the analytical case of a finite elastic body with a known crack path. This simple example introduces the core principles of path-following methods in fracture mechanics, serving as a foundation for more complex scenarios. We then address cases where the crack path is unknown a priori, requiring adaptations of the methodology to integrate numerical tools for elastic solutions, Stress Intensity Factor (SIF) computation, and crack propagation solution. Finally, we present the determination of the equilibrium path using phase-field fracture models, employing an extension [2] of arc-length methods.

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Minisymposium FS:

Fracture across the scales

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A numerical methodology for unravelling the influence of surface roughness on the fatigue life of materials

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ABSTRACT

The determination of fatigue life stands as a critical aspect in assessing the service life of off-shore wind structures and similar engineering structures. It depends on many factors, including applied loads, environmental conditions, and structural geometry, being the surface roughness a significant contributor. While an extensive literature has covered the correlation between fa-tigue life and surface roughness through empirical relationships based on large experimental campaigns, only a limited number of works have addressed the development of computational tools capable of numerically predicting this relationship, all of them based on large and costly microscope observations. However, tackling this research challenge holds immense potential in reducing the design and maintenance costs of these structures. In this context, we present an innovative approach utilizing the Phase Field fatigue model [1,2] together with stochastic tools for the development of roughness profiles [3] to unravel the intrinsic relation between fatigue life and surface roughness, providing an initial guide in the design of fatigue structures.

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The atomic-scale origins of liquid metal embrittlement in the Fe-Zn system

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ABSTRACT

Liquid metal embrittlement (LME) refers to the reduction in ductility and toughness of a solid metal when in contact with liquid metals. This kind of material property degeneration poses a serious challenge for several industrial sectors, including the automotive industry. There, the embrittlement of advanced high-strength steels by their liquified Zn-coating during welding is of major concern. This makes Fe in contact with liquid Zn a highly relevant example of an LME-susceptible metal couple.

To aid the elucidation of the atomic-scale origins of LME, we establish an atomistic simulation framework for the assessment of fracture processes (brittle and ductile) along general grain and phase boundaries as well as in generally oriented single crystals [1]. This framework takes the form of a K-test molecular dynamics (MD) setup [2] for interfacial cracks. The simulation domain, i.e. the near-crack tip region, is constructed using the Stroh formalism [3] — an approach from linear elasticity theory for modelling cracks along arbitrarily oriented dissimilar anisotropic interfaces.

The second crucial ingredient for reliable predictions of material properties, using MD approaches, is the choice of a suitable interatomic potential (IAP) to describe the interaction between the system's atoms. For our studies, we are developing a new machine-learning (ML) IAP for the Fe-Zn system, based on the atomic cluster expansion (ACE) [4] method, since the resulting potentials feature a superior combination of accuracy and evaluation speed [5].

Three main stages of the development process have to be considered. The first one is the establishment of a suitable DFT database of relevant Fe-Zn configurations. To be able to simulate LME accurately, this database also has to include fracture-related configurations.

The second stage is the training of the ML IAP, which includes hyperparameter optimisation to obtain a good balance between accuracy and evaluation speed. In the final testing and validation stage, not only fitting-specific error measures like energy and force RMSE-values are considered but also the error in predicting relevant (physical) material properties. To substantiate the testing and validation, the extrapolation grade [6] is assessed alongside the mentioned error measures to check whether or not all relevant configurations were included in the training database and learned correctly.

Finally, the application of the overall framework for investigating LME at the atomic scale is discussed. Using the fully validated K-test framework in conjunction with the newly developed Fe-Zn ML IAP, we assess the competition between brittle (crack extension) and ductile (dislocation emission) and how it is influenced by the presence of Zn at the crack tip. These atomic-scale insights will subsequently be used to formulate a predictive theory on LME in the Fe-Zn system and to inform higher-scale approaches and methods, e.g. the phase field method.

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Nano-Scale Size Effects on Stress Intensity Factors and Crack Interactions Using a Reactive Molecular Dynamics Approach

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ABSTRACT

The stress intensity factor (SIF) is a critical parameter in fracture mechanics that characterizes the stress field near the crack tip. While closed-form SIF solutions for various configurations are available in fracture mechanics handbooks or can be readily computed using numerical methods, they often overlook size effects, which might be significant at micro- and nano-scales. Analytical studies, such as those based on nonlocal elasticity theories, have demonstrated that the SIF can be size-dependent. The findings in [1] reveal that cracks in nanobeams exhibit SIFs that deviate from the predictions of classical continuum mechanics-based fracture theories.

This work examines the impact of nano-specimen dimensions on SIFs and crack interactions using a reactive molecular dynamics (MD) approach. Brittle fracture in amorphous silica under mode I and mode II loading is modeled with the state-of-the-art ReaxFF reactive force field. SIF values are computed using two distinct global and local methods: (1) a discretized atomistic J-integral approach [2], where the J-integral is calculated as a summation over three-dimensional discrete regions; and (2) crack tip stress field analysis, previously validated for silica fracture toughness in [3]. The results are compared with classical SIF solutions to uncover size effects and their implications. Furthermore, examples of size-dependent crack interactions at the nano-scale are presented, with a focus on crack tip shielding and amplification mechanisms. These phenomena are analyzed using load-displacement curves obtained from MD simulations of parallel edge cracks under tension.

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The effect of crack tip dislocation emission on toughness: A discrete dislocation dynamics study

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ABSTRACT

There is a mismatch between indicators of ductility at the atomic scale and at the micron-scale, and no clear scale-bridging between these two scales. This poses an open challenge in predicting and addressing outstanding embrittling phenomena such as hydrogen embrittlement of metals or liquid metal embrittlement, which originate from the atomic-scale interactions of impurities (e.g. hydrogen) with the crystal lattice, and result in macroscale fracture.

On the one hand, in the context of molecular dynamics (MD) simulations of crack propagation, it is customary to investigate the competition between intrinsically ductile vs brittle behavior by means of atomistic mode-I "K-test" simulations, whereby dislocation emission from a crack tip in an otherwise pristine crystal indicates ductile response, whereas atomistic cleavage indicates brittle behavior [1]. Yet, several orders of magnitude separate the atomic-scale energy-release rate from micro-scale fracture toughness measurements [2]. On the other hand, at the microscopic scale, existing discrete-dislocations (DD) frameworks enable to assess toughness by computing the R curve, yet they typically neglect the process of blunting due to dislocation emission and attribute toughness to (pre-existing) dislocation plasticity relaxing crack-tip stress fields.

In order to assess the potential relevance of dislocation emission for microscale toughness and scale bridging, we extend an existing DD plasticity framework [3] and study the competition between cleavage and dislocation emission in the presence of a pre-existing dislocation distribution around the crack tip [4]. Crack propagation is described using a nonlinear cohesive zone model inspired by the universal binding law. Crack-tip dislocation emission (CTDE) is implemented and its influence on the R-curve is considered. Our findings show that dislocation emission can result in a significant increase in the slope of the R-curve, due to crack-tip shielding caused by the emitted dislocations. Thus, intrinsic ductility can enhance the crack-growth resistance and the fracture toughness.

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Machine-Learned Interatomic Potentials for Multiscale Modeling of Fatigue Crack Growth in Aluminium Alloys

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ABSTRACT

Atomistic simulations have long been used to investigate fracture in metals, but they traditionally rely on empirical interatomic potentials, such as embedded atom method (EAM) [1]. While these potentials lead to efficient calculations, they often lack the flexibility to accurately capture the complex interactions in alloy systems, limiting their predictive capability for fracture behavior. This limitation is particularly pronounced in additively manufactured (AM) alloys, where microstructural complexity plays a key role in crack propagation. To overcome these challenges, we apply machine-learned interatomic potentials (MLIPs) to improve the flexibility of atomistic modelling.

We first employ MLIPs to reproduce quasi-static fatigue crack growth simulations in pure aluminium, benchmarking against results obtained with EAM potentials [2]. MLIPs can achieve quantum-mechanical accuracy while maintaining computational efficiency, allowing us to extend these simulations to more complex alloy systems. We then apply MLIPs to an AM aluminium alloy, performing quasi-static simulations. This approach enables us to capture atomistic fracture mechanisms while illustrating the advantages of MLIPs in modeling the microstructural effects specific to AM alloys.

By demonstrating the capability of MLIPs in fracture simulations across different aluminium alloy systems, we highlight their potential for bridging atomistic and higher scale descriptions of fracture.

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Atomistic simulations of fracture with machine learning interatomic potentials

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ABSTRACT

Simulations of fracture present a very challenging problem for atomistic modeling. Empirical interatomic potentials are often unable to describe the bond breaking mechanisms even qualitatively and their predictive power is therefore limited. Recent advances in machine learning interatomic potentials (MLIPs) have opened new possibilities to carry out simulations of realistic multicomponent systems with accuracy approaching that of electronic structure methods. In this work, we will present applications of MLIPs in fracture simulations. The main focus will be given to models based on the atomic cluster expansion (ACE), which provides a general and mathematically complete representation of the properties of interacting atoms that fulfils fundamental physical invariances and equivariances. Existing ACE models for elements as well as multicomponent systems have been shown to offer superior accuracy while remaining highly computational efficient. We will demonstrate that ACE models are able to capture accurately processes occurring at crack tips in distinct classes of materials with different types of chemical bonding.

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Minisymposium FMM:

Fracture in metamaterials

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Numerical Investigation of Rate and Scale Effects in Architected Metamaterials under High-Rate Loading Conditions

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ABSTRACT

The introduction of advanced manufacturing technologies has made architected metamaterials widely available for use in a variety of applications. Of these applications, impact mitigation in sports, space, and military contexts is of particular interest. Herein, rapid loading regimes may lead to both material and geometric nonlinearities. While the behavior of architected materials in static conditions has been widely documented, the dynamic response remains largely unexplored. In the dynamic regime, investigations tend to focus on the global response of the structure for impact mitigation [1]. However, the meso-structure of the architected material has been shown to exert a significant influence on the overall response [2].

To ensure informed design decisions in impact mitigation, it is of paramount importance to consider the dynamic response of architected materials for protection purpose. Experiments are constrained to recording the global response. Computational tools, however, facilitate insight into the processes at meso-scale of architected materials. In particular, the collapse patterns of individual truss members and their effects on the surrounding material are of interest to assess load spreading and transmission characteristics. Numerical tools allow investigation of the local loading conditions of each member of the structure and the subsequent effects on the global protection efficacy of the structure.

This research examines the influence of varying loading rates on architected materials of different geometries and meso-scale structure sizes, employing the use of structural finite elements. To this end, the algorithmic aspects are first presented, along with relevant numerical examples that demonstrate the capabilities of the model. Subsequently, the investigated architectures are described. A comparison of these structures in a static context is established, and the effects of different loading rates on the response as well as local and global collapse patterns are presented. The scaling of the internal structures and subsequent changes in collapse patterns are investigated, and the interplay between geometric structural scaling, loading rate, and plastic deformation is analyzed.

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The effect of disorder on the resistance to crack propagation of planar lattice materials

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ABSTRACT

Metamaterials have been predominantly designed with a regular and periodic topology. While this is optimal to maximise stiffness and strength, it is not necessarily ideal for toughness. Natural materials, such as wood and bone, are light and have a remarkably high toughness. They are porous, like metamaterials, but their architecture is irregular and somewhat disordered. Therefore, this work aims to quantify how disorder affects the resistance to crack propagation of metamaterials.

Current numerical techniques to predict the resistance to crack propagation (R-curve) of lattices are very time-consuming since they either require an incredibly large domain [1] or laborious manual post-processing [2,3]. In addition, these existing methods rely on the coordinates of deleted elements to compute crack growth, which would be inaccurate for disordered lattices where diffuse damage is expected. Here, we propose a new computational method to overcome these challenges. Our approach relies on the elastic strain energy to infer the current crack growth. In addition, the total strain energy is used to calculate the J-integral throughout the simulation. Using standard energy outputs streamlines post-processing and makes this approach faster than existing methods [1-3].

Our modelling approach is first validated against existing results for regular hexagonal and triangular lattices [1,2]. We then use this technique to quantify the effect of disorder on the R-curve of both hexagonal and triangular lattices. Here, disorder is introduced in the form of misplaced vertices, as well as variations in nodal connectivity and bar thickness. Work continues to identify which form and what degree of disorder can have a beneficial effect on the resistance to crack propagation.

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Designing Damage in Maxwell Lattices to Increase Toughness
8th International Conference on Computational Modelling of Fracture and Failure of Materials and Structures – CFRAC 2025

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ABSTRACT

Designing mechanisms of damage in metamaterials proves difficult due to the numerous influencing parameters and many interacting length scales. However, in structures such as Maxwell lattices, robust topology and geometry-dependent parameters dominate stress concentrations, providing a methodology for architecting the fracture paths themselves [1] and therefore the fracture toughness.

The robust mechanisms of damage in Maxwell lattices arise from the localisation of surface *floppy modes* and *states of self stress* (SSS), whose location and form can be manipulated through a topological mechanical polarisation related to the underlying unit-cell geometry [2]. By combining topologically distinct lattices the damage path can be manipulated to increase the fracture toughness and we show this experimentally and numerically for a mode I type loading setup in this study. The increased toughness is related to the fracture path length, whereby following the initial damage which removes the SSS within the lattice, the energy required within the second phase of damage can be manipulated through this length. These insights provide a simple yet robust design methodology that can be applied to tune the fracture toughness of lattices through the precise control of their damage mechanism.

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Modeling fracture of 2D architected lattices

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ABSTRACT

The fracture of architected lattices is commonly studied under quasi-static loading conditions. It is known from continuum fracture mechanics that inertia governs fracture, especially in brittle materials. However, the quasi-static assumptions neglect inertial effects on fracture, and the dynamic effects on metamaterial fracture remain moot; for example, the influence of geometry on dynamic crack propagation. In quasi-static cases, geometry plays an essential role in the fracture behavior of these materials. The fracture toughness depends on the topology and scales with relative density and lattice size [1,2]. In addition, changes in geometry away from regular lattices alter the fracture loci and toughness [3-5]. The influence of inertial effects on the fracture of architected materials and the link between geometry and fracture behavior in the dynamic scenario remains unexplored. This work presents an initial investigation into crack propagation in architected lattices under dynamic conditions. We consider regular two-dimensional architected lattices modeled as Timoshenko beams by means of finite-element analyses of the pre-cracked specimens. We offset the dynamic with quasi-static conditions as the means of comparison, varying the relative density to evaluate its influence on the crack path and inertial response.

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Efficient Prediction of Anomalous Crack Growth in Beam-Based Architected Materials via a Quasicontinuum Method

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ABSTRACT

The mechanical behaviour of periodic architected materials (or metamaterials)—including their stiffness, wave dispersion, and viscoelastic and plastic deformation—has been extensively studied and simulated. Their fracture behaviour, however, remains a subject of study and a source of surprise—even in the simplest case of a brittle base material. An example is the stable crack-growth phenomenon reported by Shaikeea et al. [1] in a three-dimensional octet lattice composed of nearly ten million unit cells and modelled using around 20 billion degrees of freedom in ABAQUS, where each strut was discretized by Timoshenko beam elements. Unlike in classical homogeneous solids, crack growth in beam-based architected materials is solely based on the simple question: which beam fails next? This discrete nature of failure and associated size effects explain the anomalous crack-growth and reported pseudo-ductility.

These large-scale simulations highlight the need for advanced computational techniques to analyse—and eventually exploit—fracture in beam-based architected materials more efficiently. Although multiscale techniques have successfully predicted the (non)linear and plastic behaviour of these materials, classical homogenization methods rely on the assumption of a separation of scales. This assumption breaks down in the case of fracture, where the fields of interest near the crack tip vary on the same order of magnitude as the size of individual beams. To overcome this limitation, we present a discrete-to-continuum technique, i.e., a quasicontinuum (QC) method, extending the work of Kraschewski et al. [2]. Each strut in our QC framework is represented by a corotational beam formulation, with cross-sections discretized into fibres [3]. A thermodynamically consistent incremental variational approach is applied at the fibre level, enabling accurate modelling of inelastic responses of base materials typically used in additive manufacturing. Our QC framework adaptively refines regions of interest—such as the crack-tip neighbourhoods or plastic zones—while applying a coarse-graining technique in less critical regions. This approach captures significant nonlinearities and localization effects in fully-resolved regions while maintaining computational efficiency.

We demonstrate that this framework enables efficient predictions of crack-propagation paths in various topologies with elastic and plastic constituent materials. Inspired by polymer networks [4], we further investigate toughening mechanisms and their influence on crack-propagation in multi-material lattices.

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Image-based tracking of the crack propagation within irregular lattices

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ABSTRACT

Architected materials offer disruptive opportunities to combine low density with high toughness or strength. Tuning their architecture allows for further unlocking of features not intrinsic to the base material, such as negative Poisson's ratio, local toughening, and ultra-stiffness [1, 2]. Due to the high slenderness of lattice struts, it is challenging to characterize how engineering the topology alters the local stress state and modifies the macroscopic failure of functionalized architected materials.
We propose an approach based on digital image correlation (DIC) to unravel the crack initiation and propagation mechanisms of 2D heterogeneous lattices under mode I loading. To identify the dominant strut failure modes, we 3D-printed compact tension specimens with stretching and bending-dominated topology (triangular, hexagonal, and Kagome). Using FE-based DIC, we measured the nodal displacements of the joints and extracted the strain distribution within the struts by sub-lattice scale meshing. Based on the gray level residuals, we determined failure criteria for the strut in terms of strain thresholding, and we tracked the crack tip advancement during testing. The critical stress intensity factor and energy release rates were obtained by a priori knowledge of the detected crack path and integrated DIC.
Leveraging these local measurements, we assessed the influence of heterogeneities on the lattice strain distribution and thus damage nucleation and propagation mechanisms, resulting in increased work to failure. Ultimately, we highlight how image-based characterization approaches enlighten the effects of the topology alterations on the fracture behavior of lattice materials and provide realistic failure criteria for damage modeling. This insight is essential to design architected materials with engineered properties and customized fracture for real-world applications.

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Minisymposium HPC:

HPC - High-Performance-Computing in the simulation of damage and fracture

Organized by G. Guillamet, I. A. Rodrigues Lopes and L. Noels

Damage multi-scale simulations with a machine learning based surrogate

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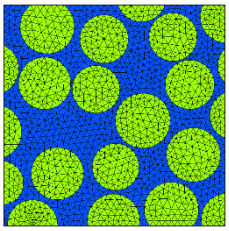
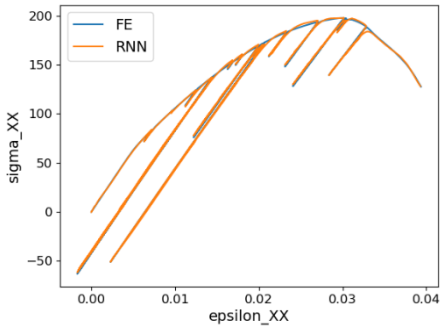
ABSTRACT

In this work, a setting to perform simulations at the macro-scale level with damage with a machine learning based surrogate of the meso-scale response is proposed.





The machine learning surrogate used is a Recurrent Neural Network (RNN), which is a kind of neural network which can handle history-dependent relations. More specifically, a RNN cell independent to the increment step (called SC-MRU-T) developed in [1] for elasto-plastic behaviours was used. A database of damaging RVE random and cyclic loading paths was built in 2D to train the RNN.

The simulations with damage are challenging because after an initial phase in which the damage is diffuse, there is a localization of the damage in a thin band which is dependent on the mesh size. To circumvent this problem, a non-local formulation that embeds the machine learning based surrogate predictions was developed in order to recover the solution uniqueness.

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Self-consistency Reinforced Recurrent Neural Networks acting as surrogates of highly-nonlinear composite responses in multi-scale simulations

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ABSTRACT

Data-driven approaches allow accelerating multi-scale simulations: the micro-scale problem resolution is substituted by a surrogate model trained from off-line simulations. In the context of history-dependent materials, recurrent neural networks can act as such a surrogate, see e.g. [1], since their hidden variables allow accounting for irreversible behaviours.

This however requires a training dataset that virtually covers all the possible strain-stress state evolutions encountered during the online phase. This dataset size can thus become prohebitive in particular when the strain increment size is expected to vary by several orders of magnitude. This is typically the case for highly non-linear problems such as the ones involving damage and or fracture since the time step size can be reduced during the on-line stage. Self-Consistent recurrent networks were thus introduced in [2] to reinforce the objectivity of the neural network predictions with respect to the strain increment size.

Nevertheless, when considering a composite representative volume element response in the context of multi-scale simulations, a Self-Consistent recurrent network might require a long training process. We have thus revisited the Self-Consistent recurrent unit in order to improve the training performance and reduce the number of trainable variables for the neural network to act as a composite surrogate model in highly nonlinear multi-scale simulations, including in the case of damage and fracture.

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Stochastic Deep Material Networks as Efficient Surrogates for Composites & Deep Material Networks performance for damaging processes

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ABSTRACT

Deep Material Network (DMN) is a homogenisation method that incorporates analytical homogenisation solutions and material constitutive relations into a neural network model yielding mechanistic building blocks [1]. DMN was reformulated from the interaction view-point [2] in order to improve its training performance.

In this work, on the one hand, the phase volume fraction is decoupled from the topological parameters of the Interaction-Based DMN (IB-DMN). Since the phase volume fraction is no longer influenced by the topological parameters, a stochastic IB-DMN is constructed by introducing uncertainties to the topological parameters of a general IB-DMN trained with linear elastic homogenization data. The nonlinear predictions of the proposed stochastic IB-DMN are compared to those from Direct Numerical Simulations (DNSs) on 2D Stochastic Volume Elements (SVEs) of unidirectional fiber-reinforced matrix composites under a finite strain setting.

On the other hand, damage is introduced in the matrix constituent phase in order to test the performance of the IB-DMN upon softening.

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Fatigue lifetime analysis of general 3D crack configurations using H-matrix accelerated boundary element method

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ABSTRACT

This work is motivated by the industry's need for an "intermediate" computational tool devoted to fatigue lifespan assessment of general 3D crack configurations, delivering an accuracy better than semi-analytical approaches (which are fast but too-imprecise except for unrealistic canonical configurations) while performing faster than full-fledged finite element analyses of complete aerospace structures or parts (whose application on real configurations sometimes involve weeks-long computations as well as labor-intensive detailed modeling).

Applying the boundary element method (BEM) [1,2] in the framework of classical 3D linear elastic fracture mechanics (LEFM) permits a reasonable compromise between physical completeness and analysis time computation, as is witnessed by abundant published literature spanning decades [3]. The BEM is well known (under the adopted LFEM framework) to allow model dimension reduction, albeit at the expense of discretized models featuring dense matrices. To avoid the latter potentially fatal computational bottleneck and thus allow 3D cracked configurations of unlimited geometrical complexity while keeping analysis time and memory in check, we implement and demonstrate a fast BEM version based on hierarchical matrix (H-matrix) compression, which achieves both substantial memory reduction and linear solver acceleration for given BEM model size. This will allow the target industrial applications to benefit from traditional strong points of the BEM in LEFM, such as accurate stress intensity factor evaluation and ease of remeshing in fatigue crack propagation analysis.

In this work, which constitutes a first stage in a longer-term industry-driven research project, we will present the above-outlined computational methodology and demonstrate its effectiveness on 3D configurations involving fatigue crack growth simulation. Further work will then aim at including this treatment into analysis of complete aerospace structures, first by using ambient stress fields yielded by FEM analysis of the uncracked structure, then by developing BEM-FEM coupling approaches, and by including a thermal gradient.

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Super-computer Implementation of the Phase Field Method to Fracture for Billion-degrees of Freedom Simulations in Heterogeneous Structures

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ABSTRACT

An efficient parallel implementation of the phase field method [1] for brittle crack simulation able to run on supercomputers with a large number of processes is proposed. This framework uses the finite-element method on 3D structured meshes and was developed for distributed memory machines using the Message Passing Interface (MPI) [2] for workload distribution and data communication between processes. Parallel assembly is carried out to build the matrices associated with the linear systems of equations. In the proposed context, linear systems derived from displacement and damage discretizations are solved using parallel solvers and preconditioners from the PETSc (Portable, Extensible Toolkit for Scientific Computation) library [3]. All additional operations in this implementation are also efficiently parallelized. Performance analysis shows linear acceleration with an efficiency of 97% for a computation on 6400 processes and over 80% for a computation on 10240 processes. The linear systems involved in the simulations with up to 10^{10} degrees of freedom can be solved in a few seconds. The methodology is applied to brittle simulations, involving alternate solving of large linear systems and incremental evolution. The applications presented to illustrate the parallel framework involve crack initiation and propagation in strongly heterogeneous materials with a detailed description of the microstructure. Large three-dimensional periodic structures and a realistic geometrical model directly obtained by micro-CT imagery are used.

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Evaluation of different continuum damage models in low velocity impact events and the importance of using high-performance computing

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ABSTRACT

The modeling of Low-Velocity Impact (LVI) events in fiber-reinforced materials is still one of the most complex and challenging problems today. In these cases, both the contact algorithm and damage model are crucial for accurately predicting the various damage mechanisms occurring beneath the impactor and ensuring the completion of the simulation analysis. Moreover, this problem is computationally demanding due to the presence of contact and the use of complex constitutive damage models, both of which require refined meshes to obtain accurate predictions. Therefore, employing High-Performance Computing (HPC) frameworks is desirable for faster time step processing and reducing the overall time-to-solution for these problems [1]. In this work, the performance of a state-of-the-art continuum damage model [2] for predicting intralaminar damage coupled with a cohesive zone model for delamination is investigated. The evaluation is first conducted in open-hole tension tests and then, for plates submitted to low-velocity impact events. The damage model has been enhanced to suppress spurious matrix cracking when fiber damage occurs [3] and to also gain robustness in LVI problems. The different damage model versions have been compared and discussed. Two different solvers are used: the first is Abaqus/Explicit, a well-established commercial software coupled with VUMAT user-defined subroutines and the Digimat modeling platform from Hexagon; the second is Alya Explicit, a parallel computational mechanics research code designed for HPC systems. The numerical predictions from these solvers and the different versions of the damage model are correlated with experiments and the computational performance is assessed, highlighting the importance of using HPC in solving computationally intensive problems related to damage, such as impact events.

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Generation of databases of anisotropic strength values from fibre-reinforced composites microstructures with high-performance-computing

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ABSTRACT

Many structural components employed in the transportation industry rely on composite laminates, which are subjected to complex loading conditions. The structural integrity of composite structures is dependent on their microstructure. Therefore, the design of such structural components aided by simulation must consider the underlying micro-mechanisms.

In high-fidelity micro-mechanical numerical models of composite materials, the fibres and the matrix geometry, along with their individual responses, are modelled explicitly. Even though this kind of models is not suitable for the direct finite element simulation of structural details due to their computational cost, they can provide important insights on the micro-mechanisms that lead to the onset and evolution of fracture in composite materials, as these result from the interplay of complex multi-scale phenomena [1]. Moreover, employing the concept of computational homogenisation, micro-mechanical models can be employed to determine ply-based properties and build databases of homogenised responses for data-driven surrogate models [2].

In this contribution, a high-performance-computing pipeline is implemented for the generation of homogenised ply-strength properties, towards the development of a machine-learning model that can predict those properties from microstructural descriptors. Sensitivity analysis on the parameters that play a major role in the obtained properties will be performed, providing guidelines for the selection of those descriptors.

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Uncertainty Quantification of Defects in Composite Structures Using High-Fidelity Simulations and HPC Resources

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ABSTRACT

The increasing use of composite materials in lightweight, high-performance structures requires robust methodologies to account for manufacturing imperfections that can compromise structural reliability [1]. This study presents an advanced uncertainty propagation framework to assess the impact of material variability and geometric defects, such as gaps, on design allowables using high-fidelity simulations and Monte Carlo methods within a high-performance computing (HPC) environment [2]. Three scenarios are analyzed under tensile and compressive loading conditions: pristine structures with material property uncertainties, structures with geometric gaps (including variations in gap width, ply location, and distance from the center), and a combination of material variability and geometric gaps.

A total of 8,500 simulations were executed using the PyCOMPSs workflow environment and the COUPONtool to systematically evaluate the influence of these uncertainties. Results demonstrate that combined uncertainties significantly reduce design allowables, with gaps having a minimal impact on tensile strength but a more pronounced effect under compressive loading. This discrepancy highlights the sensitivity of structural performance to defect types and loading conditions.

By leveraging HPC resources (RES: IM-2024-1-0027), this methodology ensures accurate, scalable, and efficient evaluations of uncertainty effects on composite structures. The findings underscore the importance of accounting for material and geometric variability in design processes to enhance structural robustness and reliability.

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Machine Learning-Accelerated Predictions of Design Allowable of Composite Laminates

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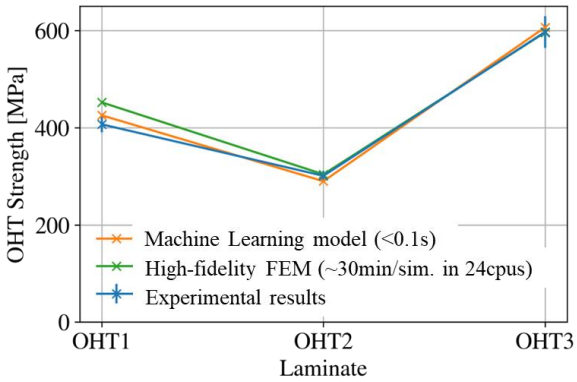
ABSTRACT

The generation of design allowables for composite laminates is of utmost importance for the design and certification of the composite structures used in the aerospace industry. The determination of these design allowables, usually relies on expensive and time-consuming experimental test campaigns. With the increase of computational power, and the development of high-fidelity numerical models that accurately represent the response of composite materials, alternatives to generate design allowables based on finite element simulations have also been sought out to reduce the certification costs. However, these solutions are still computationally expensive. The recent advances on machine learning techniques opens a new window of possibilities for the faster prediction of the structural response of materials, by allowing the definition of surrogate models that continuously and analytically describe the design space [1].

In this work, a database of open-hole high-fidelity simulations [2,3] is generated using a HPC framework and used to train machine learning algorithms, resulting in surrogate models that are able to predict the notched strength of several materials, layups and notched geometries.

The trained machine learning algorithms are shown to be able to predict the strength of open-hole multidirectional composite coupons with the precision provided by high-fidelity simulation in milliseconds, corresponding to a time-to-prediction speed-up of over 10k times.



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Physics and Sensitivity Analysis guided Active Learning for Uncertainty Propagation in High Dimensional Composite Damage Modeling

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ABSTRACT

Uncertainty propagation is a crucial step in the design and certification of composite materials. Propagating the uncertainty from input parameters to the quantity of interest can be done through the definition of a surrogate model trained on a limited number of high-fidelity Finite Element (FE) simulations. In general, collecting training data in an efficient way for a high dimensional problem can be challenging in the sense that we need to avoid sampling from non-sensitive dimensions, while focusing the available resources on the sensitive ones. This indicates that sensitivity analysis is an essential part of the equation. However, given that the problem is composites related adds an extra complexity; simulating the various failure mechanisms that interact before the final failure of composite structures is quite challenging. In fact, obtaining converged solutions may be unlikely for certain input combinations, but this cannot always be anticipated in advance. Therefore, simply rejecting these simulations does not change the fact that they represent wasted computational resources. This makes any considerable methodology that is after efficient sampling for such problems must be aware of these challenges. Under the framework of active learning, we propose an algorithm that deals with the exploration-exploitation dilemma to perform an efficient sampling for training and testing a surrogate model, which is used for the sake of uncertainty propagation. We combine two main resources: First, physics knowledge about the constrains regarding input combinations to decrease the chance of running physically meaningless FE simulations. Secondly, the predictive distribution of the surrogate model that assists in performing sensitivity analysis to guide exploration, in addition to estimating the prediction error, which guides the exploitation aspect. The data generated for training and validating the algorithm are obtained from FE simulations using advanced progressive damage models to predict the onset and progression of the different failure mechanisms. Results show that the proposed methodology is able to identify the sensitive parameters as well as train a well performing surrogate model with a moderate computational effort.

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