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Edited by:

M. Jirásek, O. Allix, N. Moës and L. De Lorenzis

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CFRAC 2023:
The Seventh International Conference on Computational Modeling of Fracture and Failure of Materials and Structures

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Preface

The series of International Conferences on Computational Modeling of Fracture and Failure of Materials and Structures (CFRAC) started in Nantes in June 2007 and continued in Barcelona (2011), Prague (2013), Nantes (2017) and Braunschweig (2019). After an interruption caused by the coronavirus pandemic, the seventh edition of CFRAC is held at the Czech Technical University in Prague on 21–23 June 2023. Its scientific program consists of 5 plenary lectures and 45 parallel sessions assembled into 14 minisymposia, in which 12 keynote lectures and about 200 regular lectures are given. Each lecture is represented in this proceedings book by an abstract. In addition, a special fracture benchmark will be presented and discussed in 2 sessions.

CFRAC belongs to the large family of ECCOMAS Thematic Conferences, organized with the support of the European Community on Computational Methods in Applied Sciences. The purpose of CFRAC is to bring together academic researchers and industrial partners involved in the development and application of numerical procedures for fracture and failure simulation of materials and structures.

The growing need for efficient and robust numerical methods dealing with fracture and failure can be attributed to the fact that designers of engineering structures must respond to ever increasing demands on performance in terms of safety, reliability, durability, low cost and low energy consumption. As new materials and new applications emerge, traditional design rules and conventional testing methods become insufficient or inapplicable, which strengthens the role of computational methods in the design process. Numerical tools can substantially accelerate the development of new products and their optimization. The ambition of CFRAC conferences is to serve as a platform for presentation and discussion of exciting advances in various branches of computational fracture and failure mechanics, and to promote collaboration among research groups in Europe and worldwide.

One of the characteristic features of the CFRAC series of conferences is the emphasis on a participant-friendly environment, encouraging the presentation of the most recent results. For instance, the final deadline for submission of contributions to CFRAC 2023 was just four months before the actual conference, and the authors had the opportunity to update the abstracts even later. Only short abstracts were required and the authors retain the copyright. At the conference, at most six sessions run in parallel, in lecture rooms located next to each other. The coffee break refreshments and the lunches are served in one spacious lobby, so that the participants can remain together and continue their discussions in a relaxed atmosphere. The organizers believe that such conditions facilitate the exchange of ideas and contribute to the success of the conference.

The present proceedings volume has been assembled from individual abstracts submitted by their authors. The final unified pdf file with a table of contents and author index has been processed by Michal Šmejkal, a doctoral student at the Czech Technical University in Prague. We would also like to thank the minisymposia organizers and the plenary speakers and acknowledge their important contribution to the preparation of CFRAC 2023.

Finally, let us mention that the complete proceedings can be freely downloaded from the conference web site via `http://mech.fsv.cvut.cz/cfrac/proceedings2023.pdf`. We hope that the readers will find here stimulating ideas and enjoy the reading.

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- Vikram Deshpande, University of Cambridge, UK
- Jay Fineberg, The Hebrew University of Jerusalem, Israel
- Peter Grassl, University of Glasgow, UK
- Varvara Kouznetsova, Eindhoven University of Technology, The Netherlands
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- Peter Wriggers
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Plenary Lectures

Supershear cracks in Tensile Fracture: How fast can materials break?

Meng Wang, Songlin Shi, and Jay Fineberg

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Brittle materials fail by means of rapid cracks. At their tips, tensile cracks dissipate elastic energy stored in the surrounding material to create newly fractured surfaces, precisely maintaining `energy balance' by exactly equating the energy flux with dissipation. Using energy balance, fracture mechanics perfectly describes crack motions; accelerating from nucleation to their maximal speed of c_R the Rayleigh wave speed. Beyond c_R , tensile fracture is generally considered to be impossible [1], [2].

Recently, the potential emergence of an entirely *new* branch of fracture *not* incorporated in classical fracture mechanics has been predicted in lattice models to occur at high applied stretch [3]–[5]. This theory predicts Mode I cracks that are able to exceed the shear wave velocity, c_s, and potentially even the dilatation waves speed, c_P [6], [7]. Moreover, these new fracture states are not expected to be governed by the principle of energy balance, the cornerstone of the classical theory of fracture.

Experiments have observed marginal supershear propagation in rubber [8] under extreme (200-300%) strains, however unequivocal experimental evidence for supershear tensile fracture has long been lacking. Here, by the use of brittle hydrogels, we experimentally demonstrate that such a wholly new and different class of tensile cracks indeed exists. We demonstrate that the principle of energy balance no longer dictates their dynamics; this new branch of cracks smoothly surpasses c_R to reach unprecedented speeds that approach the speed of dilatation waves. The transition from `classical' cracks to these `supershear' cracks takes place at critical values of applied strains. We, furthermore, show that the values of these, rather moderate (12-14%), critical strains are intimately related to the microscopic material structure.

While it is still unclear whether this intriguing fracture mode is indeed that predicted theoretically by Marder [4], [9]. It is clear that these extreme tensile cracks have never before been clearly observed in experiments. This new mode of tensile fracture represents a fundamental paradigm shift in our understanding of 'how things break'.

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Fracture of microarchitected solids and their anomalous toughness

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There has been an explosion in the development of light and strong mechanical metamaterials in the past decade [1-3] reporting extreme effective properties. As rapid progress in additive manufacturing and design methodology continues to proliferate these metamaterials, their application as structural materials is ultimately limited by their tolerance to damage and defects. While significant advances have been made in reporting extreme properties such as stiffness and strength, material properties that enable us to define the tolerance of metamaterials to defects as yet remain unclear. All work to-date has a-priori assumed (and without a-posteriori experimental validation) that a material property known as fracture toughness exists for these materials akin to usual continuum structural materials. In fact, all existing experimental measurements are based on metamaterial specimens comprising only dozens to at most a few hundred unit cells where the so called "K-field" required to define an effective toughness is not established. The material properties that govern the defect sensitivity of metamaterials thus remain largely unknown.

Via a combination of additive manufactured metamaterial samples with millions of unit cells printed by a large area high resolution additive manufacturing technique, a range of loading conditions and detailed in-situ X-ray tomography all combined with very large-scale numerical simulations (in excess of 100 billion degrees of freedom) we have uncovered [4] the elusive failure mechanics of mechanical metamaterials. We have demonstrated that (i) the property known as fracture toughness is insufficient to characterise fracture and (ii) standard fracture testing protocols, established over the last 50 years, are inappropriate for such materials. The outcome is succinctly summarised in a fracture mechanism map that fully characterises the fracture of three-dimensional metamaterials under arbitrary loading conditions.

Even more intriguingly, again using a combination of dynamic X-ray tomography coupled to finite element calculations we show that metamaterials made from a purely elastic parent material display rising R-curves. These rising R-curves are not a consequence of the usual crack ductility mechanisms such as crack tip plasticity or crack bridging but rather due to an inverse elastic strain gradient effect that seems to be unique to such metamaterials. We shall discuss these inverse elastic strain gradients effects and the consequent specimen size effects wherein continuum fracture properties are not realised in metamaterials until they exceed 10s of million-unit cells. Such specimens are not only unrealistic in terms of current testing/manufacturing capabilities but also in terms of most applications. We shall end with a discussion on the analogy between the anomalous toughening of the biological metamaterial, viz. trabecular bone and these artificial metamaterials.

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A multi-scale model for interfaces with a jagged deformation and failure mechanism

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Damage initiation in many multi-phase materials can be attributed to a peculiar deformation mode, where one of the phases deforms anisotropically by forming serrated, jagged, interface impinging on another (approximately isotropic) phase. This locally induces large strain concentrations at the fine scale in the near-interface second phase, where nano-voids can form and grow, leading to damage and crack formation. Examples include twins impinging on a grain boundary [1], crystalline-amorphous interface [2] or martensite-ferrite interface in advanced multi-phase steels, where martensite islands typically deform by sliding on the retained austenite films [3].

The cohesive zone modelling is by now a well established approach for modelling interface decohesion and damage, avoiding detailed resolution of the detailed micro-(nano-)scale effects. When the interface damage mode involves pure displacement opening (normal and/or tangential to the interface), procedures for phenomenological or multi-scale identification of the cohesive zone law have been well established in the literature. However, to the best of our knowledge, interface damage resulting from the jagged sliding of one of the phase has not yet been considered in the context of interface modelling.

In this contribution, we propose a novel multi-scale, computational homogenization based approach for such interfaces. At the mesoscale, a two-phase mesostructure is considered. The kinematics of the mesoscopic interfacial zone entails an interface separation, which includes the contributions of the jagged sliding active and inactive modes. The inactive mode contribution follows the classical cohesive interface description, while the active mode is driven by the near-interface jagged deformation of the anisotropic phase, leading to an enhanced cohesive interface description. At the microscale, an interfacial zone unit cell resolving the substructure and anisotropic, discrete deformation mode is considered. To describe the formation and growth of the nano-voids in the second phase, a continuum damage model incorporating volumetric and deviatoric damage is adopted. Two effective interface separation quantities associated with the jagged deformation inactive and active modes, are defined and computed from the correlated micro-fluctuations within the interfacial unit cell. Applying the extended Hill-Mandel condition yields the generalized tractions conjugated to these interface kinematic quantities. Relating the effective quantities, leads to an enhanced cohesive law. This microphysics-based effective interface model is fully identified using a set of "off-line" representative unit cell simulations.

The developed effective interface model is numerically validated against fully resolved modelling of infinite mesoscopic interfacial zones. As an example, the model is applied to modelling interface damage in a dual-phase (DP) steel microstructure, where the model performance is validated against microscale experimental results.

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On the modelling of fracture processes in cohesive-frictional materials

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In recent experiments, it has been shown that for tensile fracture with lateral compressive stresses, the fracture energy in tension is increased considerably [1]. For reinforced concrete structures, these types of fracture processes with combinations of tensile and compressive stresses occur during shear and splitting failure modes. The effect of lateral compressive stresses on the fracture process in tension is often not explicitly considered in fracture models for quasi-brittle materials [2]. The aim of the present work is to investigate this phenomenon by means of meso-scale analyses to obtain a better understanding. Furthermore, it is aimed to investigate if the concrete damage plasticity model 2 (CDPM2) presented in [3] is capable to reproduce the effect of lateral compressive stresses on tensile fracture observed in experiments and meso-scale analyses.

For the meso-scale lattice approach, a damage-plasticity constitutive model is combined with an auto-correlated random field of strength and fracture energy [4]. Initially, the lattice approach is compared with experimental results in uniaxial tension and uniaxial compression. The results show a good agreement between simulations and experiments. Then, cells with periodic lattices and periodic boundary conditions are loaded in two steps. Firstly, compression is applied. Next, the cell is extended in the lateral direction while keeping the compressive stress constant. It is shown that with increasing compressive stress applied, the post-peak energy dissipation in tension increases. Postprocessing of the results of the analyses reveals that this increase is due to greater frictional energy dissipation and greater number of cracks than for pure tension.

The findings of the meso-scale analyses and the experiments reported in the literature are then used to investigate the response of the macroscopic constitutive model CDPM2. Special attention is paid to the ductility measures of the damage part of CDPM2 and the way the effective stresses are split into tensile and compressive parts. Then, this model is used for finite element simulations of a concrete beam failing in shear for which the results were reported in Leonhardt and Walther [5].

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On the modelling of fracture processes in cohesive-frictional materials

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Minisymposium CDP:

Cyclic damage processes in concrete

Organized by F. Aldakheel, M. Kaliske, G. Meschke, J. Schröder, H. Steeb, J. Storm and P. Wriggers

High Performance Computing for Concrete Fatigue Failure in Poro-Elastic Media

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The fatigue behavior of concrete with high moisture content has become an important subject of interest with the expansion of offshore wind energy systems. Investigations in the literature indicated that the numbers of cycles to failure significantly decreases with the increased moisture content in concrete. This work presents a novel variational phase-field model for modeling water-induced failure mechanisms due to the cyclic loading in concrete. As a key feature, the fatigue-induced fracture is formulated based on the accumulation of the bulk energy in time, and so a critical stress state (which indicates the crack initiation) will be drastically reduced [1].

These failure mechanisms are coupled to fluid flow, resulting in a Darcy-Biot–type hydromechanical model [2]. Here, the model employs a micromechanics-based theory for description of specific fracture driving state function to model compression/shear regime in concrete. As another important feature, the model includes a non-associative frictional plasticity law which is suitable for the concrete [3, 4]. Numerical results confirmed that the fatigue effect results in the reduction of the crack resistance for the water-saturated case in comparison to the dry test. So the number of cycles to failure for both dry and fully saturated cases are analyzed over the degradation process.

Finally, the complete failure state of the specimen is further examined with an experimental observation to verify the proposed model. To do so, the influence of the loading frequency on the fatigue behavior of concrete has been investigated. This has been done for both dry and fully saturated media. We observed that the failure of high concrete moisture contents is more pronounced for lower load frequencies. This is further investigated through our proposed numerical formulation, and validated with experiment.

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Mixed-mode Fracture Simulation by the Phase-field Method

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The failure mechanism of rock-like materials has been of great research interest. From the experimental observations, fracture is in general anisotropic and the evolution process is rather complex, often characterized by multiple cracks initiating sequentially at different positions and orientations. Researchers often refer to this type of failure as mixed-mode failure, in the sense that anisotropic failure is comprised of at least two types of mechanisms – Mode I failure caused by tensile loading and Mode II failure by shear loading. Numerous works have reported such behavior in different materials, such as cement-based materials, marbles, gypsums etc.

In terms of the numerical description of the fracturing process, the phase-field methodology has been proven to be a promising approach during the last years. Consistent with the GRIFFITH theory on the energetic description of fracture, the approach is capable of numerically capture the nucleation, initiation, propagation and merging of cracks without additional numerical manipulations.

Recently, the phase-field model has been combined with the so-called Representative Crack Element (RCE) framework in [1]. Within the RCE, the material state is interpreted as an interpolation governed by the degradation function, between an intact state and a completely failed state. This renders physically meaningful crack kinematics, i.e. post-crack behavior including the opening and closing of the crack, as well as the shearing at the crack surface, which is not the case for most of the previously existing phase-field models. The crack-induced displacement discontinuity is explicitly considered as an internal variable, facilitating the consideration of many mechanisms at the crack surface, such as cohesive behavior and friction. In this work, the crack coordination system (CCS) that is embedded in the RCE concept, has been employed to work together with an orientation-dependency of the fracture toughness. As such, the mixed-mode phase-field model is formulated in a straightforward manner.

Following the minimization of virtual power on the RCE level, the analytical solution for crack deformation is directly obtained. Based on a consistent derivation, the finite element implementation of the mixed-mode RCE phase-field model is carried out in a straightforward manner. Several illustrative examples serve to describe failure mechanisms in the experiments.

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Phase-field modeling of failure behavior of reinforced high performance concretes at low cycle fatigue

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In the recent decades great research effort has been carried out which led to more efficient and stronger concrete types, e.g. high performance concrete (HPC) and ultra-high performance concrete (UHPC). They are rapidly emerging as promising materials in construction industries worldwide. HPCs are available in wide varieties of composition which make them different from classical concrete types. For example, steel fibers and short-wire fibers are usually added to ensure ductility in HPC and in UHPC, respectively. The fiber reinforcements provide a sufficient ductility by transmitting the stresses in concrete from matrix to the fibers during fracture. These fibers contribute to the energy absorption capacity of concrete by restraining the further growth of crack. This process shows pronounced effect on the deterioration characteristics of concrete in cyclic flexural tests, see [3].

In this contribution, the aim is to investigate the influence of fiber's orientations and distribution on the overall material behavior of fiber reinforced HPCs at low cyclic fatigue. A phenomenological material model is developed by combining the superposed models of transversal isotropic elasto-plasticity, see [1] and a continuum phase-field model of fracture in elasto-plastic material, cf. [2, 4, 5]. Two different continuous stepwise linearly approximated degradation functions for the modeling of unsymmetric behavior of concrete materials in tension and in compression are considered. The numerical model is calibrated using the experimental data and by simulating the typical uniaxial cyclic tests and three-point bending beam test at low cycle for pure concrete specimens. Three-point bending beam tests at low cycle for reinforced HPCs with different fiber contents and orientations are simulated. To incorporate the different distributions and orientations of reinforced fibers different orientation distribution functions (ODF) are constructed and implemented. The degradation of residual stiffness is calculated using experimental and numerical results and compared to validate the accuracy of the numerical results, see [5, 6].

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Mesoscale modeling of high-performance fiber-reinforced concrete under monotonic and cyclic loading

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Concrete is one of the most commonly utilized building materials and has a significant environmental impact due to the high energy needed for cement production. Over the past decades, significant progress has been made in developing high-performance and ultra-high-performance concretes and incorporating fiber reinforcements in structural concrete resulting in material savings and improved durability.

However, to fully realize the potential benefits, better models and design approaches must accompany these material improvements. This work focuses material behavior aspect of fiber-reinforced high-performance concrete, investigating damage processes and mechanisms occurring at small scales, which are not readily observable during loading tests. To this end, it presents a framework for generating mesoscale concrete models based on virtually created aggregate and fiber distributions [1], as well as from Computational Tomography (CT) images. A finite element model utilizing zero-thickness interface elements is applied to simulate the fracture behavior of mesoscale specimen models. The zero-thickness interface elements are equipped with a cohesive-frictional traction-separation law that includes dilatancy due to aggregate interlocking and a model for hysteresis occurring due to incomplete crack closure during loading-unloading cycles. The steel fibers are considered explicitly and modeled as elastoplastic Timoshenko beam elements. The 3D elastoplastic constitutive law with isotropic and kinematic hardening is adapted for beam elements by iterative solution of zero stress constraints via Newton's method [3]. The embedment of fibers into the cement matrix is facilitated via a penalty-based tying algorithm that enables flexible placement of fibers without needing to conform with the background mesh. The bond between the cement matrix and fibers is modeled via an elastoplastic bond-slip law proposed in [2], whose parameters are calibrated based on single-fiber pullout experiments. All model components are implemented into the open-source Finite Element program "Kratos Multiphysics" [4].

The capabilities of the proposed model are demonstrated by reanalyzing several experimental scenarios, such as notched prismatic specimens under uniaxial tension [5], small cylinders under uniaxial compression, and fiber-reinforced high-performance concrete beams under three-point bending and comparing results with the available experimental data.

The presentation is closed with a discussion of implementation, the benefits and limitations of the proposed modeling approach, and potential ways to improve the model further.

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Concrete fatigue modeling and experimental characterization based on inter-aggregate cumulative sliding hypothesis of degradation

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A physically rigorous modeling of fatigue-induced degradation processes in the material structure of concrete is a paramount requirement for a significant improvement of existing, empirically based design concepts, particularly for reinforced concrete structures. In our recent work, we introduced a dissipative hypothesis ascribing the key fatigue driving degradation mechanisms to a cumulative measure of inter-aggregate shear strain. The hypothesis leads to a new formulation of a pressure-sensitive interface model [2], that can be embedded both in a discrete model of a material zone or in a tensorial formulation of a microplane model. An example of a microplane formulation (MS1) [3] including cumulative sliding as a dissipative mechanism has been introduced, showing the ability to capture the fatigue-induced tri-axial stress redistribution in the concrete material structure subjected to pulsating subcritical load.

To isolate the dissipative mechanisms and to validate the model, test configurations with controllable levels of combined compression and shear fatigue load are needed to cover the design-relevant range of stress configurations in a more appropriate way than the standard cylinder test. Alternative test setups have been developed recently, introducing a modified punch-through shear test (PTST) [1]. The combined experimental and numerical studies cover a wide range of stress configurations in the test ligament of the axi-symmetric punch-through shear test. The simulation with two different fatigue load amplitudes predicted larger number of cycles to failure for the lower amplitude, qualitatively complying to the Wöhler (S-N) curve of concrete.

Due to the thermodynamic formulation of the constitutive model, the energy breakdown of the individual inter-aggregate dissipative mechanisms could be quantified for a uniform shear fatigue loading at varied levels of confinement [4]. These studies reveal that plastic energy dissipation increases for lower fatigue amplitudes of the fatigue load leading to longer fatigue life, while damage dissipation remains nearly constant for loading scenarios with different amplitudes. Such conclusions stimulate the development of engineering design concepts that can realistically capture the fatigue life of high-performance reinforced concrete structures.

In addition to the uniform fatigue shear loading, also the effect of variable load amplitude has been studied and interpreted using the model MS1. Both experimental and numerical results have shown that the currently used Palmgrem-Miner design rule is not realistic, and needs to be refined to deliver reliable predictions of structural lifetime.

Besides the smeared representation of the dissipative process using the microplane model MS1, a discrete model employing the same inter-aggregate dissipative hypothesis will be presented, providing the possibility to study the localization processes and energy dissipation patterns due to fatigue loading within a representative dissipative process zone. A possibility to establish an energetic equivalence between both models will be discussed.

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High-frequency fatigue experiment using Dynamic Mechanical testing (DMT) and in-parallel extraction of complex mechanical properties using Dynamic Mechanical Analysis (DMA)

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Due to cyclic load, fatigue affects brittle materials like (ultra) High-Performance Concrete (UHPC) used in marine and civil structures, resulting in unexpected failures. Additionally, in order to analyze mechanical properties of materials, understanding how materials respond to different frequencies is crucial for industrial designers. When a material is subjected to more fatigue cycles, its mechanical properties undergo changes. To extract material's properties under fatigue load at a specific cyclic speed, It is necessary to obtain the mechanical response of the material at the same frequency speed. Cyclic load tests are conducted to determine how fatigue affects the material and the number of cycles it will take to fail is experimentally determined. The problem with such tests is that they are potentially expensive, i.e., it could take a long time since the number of loading cycles can be extremely high. Moreover, it is not possible to observe the evolution of (micro-)cracks within the different damage phases of cycling tests. It is also challenging to characterize the material's small-strain stiffness evolution. This research aims to investigate the use of high-frequency excitation with a (large amplitude) dynamic mechanical testing (DMT) for the High Cycle Fatigue experiments and also in-parallel extraction of material properties with a (low amplitude) Dynamic Mechanical Analysis (DMA). The test setup applies excitation using high-voltage piezoelectric actuators and then the failure modes of the material will be examined. The excitation frequency for the fatigue test is between 10 and 200 cycles per second which allow for reducing the experimental investigation time to failure. Further, it allows investigation of the effect of frequency on the number of cycles to failure. In addition, the (rate-dependent) complex mechanical properties of the materials in tangential space are obtained in frequency between 0.01 Hz to 1000 Hz using direct measurement with DMA method; while, the observed mechanical properties of these materials change with increasing frequency. In the case of materials' behavior, by increasing the frequency, Young's modulus increases and Poisson's ratio decreases. Experimental fatigue results will be presented for (U)-HPC and Berea sandstone samples. Harmonic experimental data include (direct) strain measurements in axial and circumferential directions as well as forces in axial directions. In addition, the resulting complex Young's modulus and evolving damage-like "history" of HPC and Berea sandstone specimens will be shown.

An adaptive cycle-jump method to accelerate phase-field computations of fatigue

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Phase-field models of fatigue, e.g. [1, 2], proved to be a versatile approach capable of reproducing the characteristic experimental features of fatigue. However, their high computational cost makes the cycle-by-cycle analysis of components in the high cycle fatigue (HCF) regime, that is cycle counts of $n > 10^4 - 10^5$, unfeasible. One strategy to solve this issue is to employ a time acceleration scheme whose simplest form is the *cycle-jump* approach, where selected state variables are extrapolated over a certain number of cycles Δn based on an explicitly (cycle-by-cycle) computed evolution of the system.

To exploit the full potential of this procedure while keeping the accuracy of the solution, an adaptive cycle-jump algorithm is proposed for the model presented in [1] which degrades the fracture toughness of the material as a representative fatigue history variable $\bar{\alpha}$ accumulates above a certain threshold value $\bar{\alpha}_T$. The core idea of the presented acceleration technique is to decide whether to jump cycles or not and how many cycles Δn to skip based on both the phase-field d and fatigue history variable evolution. This specific choice makes the adaptation of the proposed acceleration strategy to other phase-field fatigue models straightforward.

The computation is subdivided into four main stages: (i) early stage before fatigue effects are triggered, namely until $\bar{\alpha} \simeq \bar{\alpha}_T$ for the fist time, (ii) crack nucleation stage, i.e. between the end of the first stage and the instant in which the phase field reaches $d \simeq 1$ for the first time, (iii) stable crack propagation (also known as Paris regime) and (iv) unstable crack propagation before failure. During the first stage, the system is essentially linear elastic, which can be exploited to compute how many cycles are needed to meet the condition $\bar{\alpha} = \bar{\alpha}_T$ and thus directly jump to that point. Within the second stage, the system exhibits a stable evolution of the phase field variable d until right before the complete nucleation of a crack, i.e. $d = 1$. In this case, the determination of Δn is based on the rate of change of the $L2$-norm of the phase-field $||d||_2$ with respect to the cycle count, obtained during a small number of explicitly resolved cycles. In particular, Δn is computed as the maximum number of cycles which can be skipped before the rate of $||d||_2$ overcomes an appropriate threshold. After that, the system experiences a rapid and highly non-linear behavior lasting for a limited number of cycles, which are resolved explicitly. Once this phase is over, the stable crack propagation starts which, encompassing the vast majority of the fatigue cycles in the HCF regime, offers the highest potential for accelerating the simulation. In this third stage, the computation of the number of cycles to skip is again based on the rate of change of $||d||_2$, similarly to the second stage. The monitoring of the $L2$-norm of the phase-field also allows to detect the onset of unstable crack propagation, during which the algorithm reverts to a cycle-by-cycle computation until final failure.

The proposed methodology is first investigated using different choices for its parameters and extrapolation strategies. Then, it is used to analyze the fatigue behavior of different virtual specimens. Finally, the results are compared to those obtained with a cycle-by-cycle and a fixed (i.e. non-adaptive) cycle-jump approach.

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Eigenstress-based Anisotropic Damage Modelling of Concrete at the Meso-scale

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Concrete is a complex multi-scale composite material that exhibits different mechanical behaviour at different levels, where the behaviour at one level can be explained by the structural behaviour at the lower level. At the meso-scale, concrete is typically modelled as a three-phase heterogeneous material consisting of aggregate particles, a cement mortar matrix, and a weak and very thin layer around the coarse aggregate particles, referred to in the literature as the interfacial transition zone (ITZ).

Experimental studies have shown that the microstructure of concrete has a large number of cracks before any external loading. These micro-cracks are caused by the micro-tensile stresses (eigenstresses) that develop in the concrete during the pre-loading phase due to endogenous shrinkage and drying shrinkage[1,2], as a result of mismatch of physical and mechanical parameters of adjacent phases of concrete (cement matrix, aggregate and ITZ).

The irreversible deformations observed experimentally after cyclic loading of concrete under uni-axial compression are often explained in the context of computational plasticity and the mechanics of ductile damage [3]. In this work, a new hypothesis is proposed to physically explain the permanent strains observed experimentally in cyclic fatigue of concrete. This hypothesis is based on *the release of the initial residual stress (eigenstress)* due to damage development in the elastic phase.

To examine the extent to which the presence of eigenstress may be the cause of the irreversible displacements that characterize the cyclic compressive behaviour of concrete, a continuum thermodynamically consistent elastic-brittle anisotropic damage model is implemented for the cement mortar and a three-dimensional analysis of the concrete is performed at the mesoscale considering the early damage of concrete in the pre-loading phase.

The coarse aggregates in the 3D mesostructure model are assumed to be spheres and randomly generated considering the shape, distribution and volume fraction of the aggregates. A linear elastic non-damaging material model is assigned to the aggregates. Intrinsic cohesive interface elements with zero thickness are inserted along the aggregate-cement mortar interfaces to represent the ITZ. The ITZ is associated with a bi-linear traction-separation law.

For the damage model of the cement matrix, the effective strain space is used based on the equivalent strain energy hypothesis, and a fourth-order damage effect tensor is employed to relate the strains in the effective and damaged configurations. Satisfaction of the first and second laws of thermodynamics is ensured. The Helmholtz free energy is introduced as a thermodynamic state potential that depends on the strain tensor as an observable and the internal state variables of damage evolution and damage hardening. The evolution of the conjugate thermodynamic forces is determined by the assumption of the physical existence of a damage dissipation potential. The Lagrangian minimisation approach is used to derive the laws of damage evolution and hardening for the proposed model. This model is implemented as a user-defined material subroutine (UMAT) in the advanced finite element software Abaqus. The results obtained from the mesoscopic numerical simulations are then compared with experimental observations

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Identifying the extent of shrinkage-induced surface cracking from the time-dependent deflections of concrete beams exposed to symmetric and non-symmetric drying

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The service life of reinforced concrete structures is to a considerable extent determined by the durability of the concrete cover, which protects the steel reinforcement from corrosion. This cover is subject not only to mechanical loading but also to environmental actions causing non-negligible eigenstrains with different sources. Probably the most significant phenomenon is drying shrinkage, which is approximately proportional to the decrease in relative humidity. Moisture diffusion in concrete is extremely slow and highly nonlinear, which causes steep gradients in relative humidity distribution even without severe drying conditions. Due to the internal restraint by the cross section (which remains planar), such nonuniform field gives rise to self-equilibrated stresses which are partially relieved by creep of concrete but might attain tensile strength and cause cracking.

In 2019, an extensive experimental campaign on the time-dependent behavior of structural concrete exposed to drying conditions has been initiated at CTU in Prague [1]. All samples were prepared from an identical batch of concrete and cured for one month. The key component of the program was a set of simply supported beams of various sizes ($L = 1.75 - 3.0$ m, $h = 0.05 - 0.2$ m) and several sealing setups which influenced not only the drying rate, but also the degree of internal restraint and thereby the extent of damage. Although the experiment is located indoors, the measured mid-span deflections promptly respond to seasonal and surprisingly even daily variations in relative humidity. In contrast to conventional experiments on symmetric cylinders, the measured response in bending experiments with non-symmetric drying allows to distinguish the individual components of deformation more clearly and to assess the drying shrinkage-induced damage.

Bayesian inference allows for a robust, probabilistic, and well-posed formulation of parameter identification, even for combining limited data acquired from different experimental scenarios. The probabilistic formulation provides not only a single-point estimate of the material parameters but also an evaluation of the underlying uncertainty in the estimated values reflecting the experimental error (i.e., the uncertainty in the observed quantities) on one side and also the uncertain prior expert knowledge about the parameter feasible or more probable values. The main drawback of Bayesian inference arising from its high computational requirements due to repeated FE-based simulations will be mitigated by constructing the polynomial chaos-based surrogates for simulated response quantities. As an additional advantage, polynomial surrogates provide a fast and elegant way to evaluate the global variance-based sensitivity analysis, which allows us to analyze the effect of material parameters or their specific combinations on particular observed quantities.

In this contribution, such framework uses data from coupled hygro-mechanical low-fidelity finite element simulations in program OOFEM to identify the parameters of the constitutive models, in particular the modified Microprestress-solidification theory [2] with the damage extension and the model for moisture transport proposed by Kuenzel. Finally, the computed distribution of damage and its influence on stiffness in bending is experimentally verified.

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A Three-Dimensional Constitutive Model for Low- and High-Cycle Fatigue Behavior of Concrete at the Meso-scale

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In this paper a new 3D visco-elastic-plastic damage model is proposed to describe the behavior of concrete subjected to cyclic loadings until failure. The proposed model uses a modified version of the pressure-dependent Menétrey-Willam yield surface [1] to account for damage and fatigue. Meanwhile, the viscous behavior is modelled by means of the B3 model by Bažant and Baweja, and implemented through the exponential algorithm [2]. Specifically, the damage formulation considers two damage variables to account for the different degradation processes in tension and compression, and a stiffness recovery function to account for crack-closure effects during the cyclic loadings [3]. The fatigue model is based on the assumption of the reduction of the size of the elastic-domain, by including a fatigue softening function to the Menétrey-Willam yield surface. The proposed model also allows for the assessment of fatigue accumulation within the yield surface, based on the amount of extension experienced during high-cycle fatigue. A random distribution algorithm for the placement and compaction of polyhedral shaped aggregates, in agreement with a prescribed gradation curve, is used for the solid modeling of concrete samples at the meso-scale. The effectiveness of the model is discussed based on the juxtaposition of numerical results obtained by the presented approach, and experimental ones available in literature.

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Minisymposium CSD:

Connecting scales and disciplines to model fracture

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A discrete-continuum particle method for complex deformation and fracture events

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Complex fracture events take place in many materials and applications.In this context, discrete particle methods are an attractive computational methodology since they can easily accommodate complex and arbitrary discontinuities. The added value of particle methods to capture intricate fracture behaviour of elastic-brittle materials such as glass and concrete, has been widely demonstrated in the literature. Beyond linear elasticity and the small strain fracture regime, the ability of current particle methods such as the Discrete Element Method (DEM), Smoothed Particle Hydrodynamics (SPH) and Peridynamics to account for the underlying material behaviour remains questionable. Most of the discrete constitutive formulations are not consistent with their continuum counterparts. The origin of this limitation stems from the adopted mathematical formulation that only yield approximate deformation tensors.

This contribution introduces an innovative particle method that relies on a dedicated averaging scheme that determines the deformation gradient tensor at each particle based on the relative positions of the particle's nearest neighbours [1]. The adopted scheme reveals similarities with the volume weighted nodal averaging procedure used in the Finite Element Method (FEM) [2]. The novel particle routine, referred to as the Continuum Bond Method (CBM), preserves the constitutive flexibility of continuum methods while maintaining the powerful fracture properties of discrete particle methods. Within a general context, two numerical examples are presented to demonstrate the discrete-continuum consistency and its complex fracture capabilities: (i) an elasto-plastic tensile bar subjected to large deformations and (ii) a dynamic crack branching problem. The first example relies on a finite strain J_2 plasticity model with non-linear hardening law. The local and global mechanical response obtained with CBM is assessed in direct comparison with a FEM reference solution and further compared to SPH results. The second numerical example demonstrates the CBM's capability to account for complex fracture events, which are naturally driven by the dynamics in the simulation. The need for specific criteria and tailored domain enrichments that would allow for crack branching in dynamic fracture simulations is hereby obsolete, which is one of the major merits of particle methods.

The methodology is next applied to the micro-scale scratching of mono-crystalline silicon. Two ingredients are important for this model: (i) a three-dimensional CBM implementation in LAMMPS and (ii) constitutive model that accounts for pressure-induced phase transformations in silicon (based on [3], extended to finite strains). the LAMMPS-CBM scratch setup will be used to evaluate the global and local response from a modified continuum plasticity model designed to phenomenologically capture silicon phase transitions under contact conditions. In the future, this will be extended beyond the ductile-to-brittle transition point, which can be easily achieved with CBM using a bond breakage criterion.

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Atomistics of hydrogen at defects towards a multi-scale, bottom-up theory of hydrogen embrittlement

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The quest for cleaner alternative sources is all time high and hydrogen (H) has the potential to lead this transition owing to its clean and sustainable make-up. However, the realisation of H as an energy source requires resolving the embrittling phenomenon of H in metals. Over the past decades, several different embrittlement mechanisms have been proposed following experimental and numerical investigations [1]. Nevertheless, the operating conditions of these mechanisms are not completely understood yet, especially with respect to the role of local H concentration and the interplay of H with defects such as dislocations and cracks, which dictate the overall fracture toughness.

In this work, we primarily investigate the nano/micro-scale interaction of H with dislocations and cracks in iron (Fe). We first develop a novel machine-learning interatomic potential, based on an extensive database of Density Functional Theory (DFT) configurations. We implement an active learning technique [3] in order to simulate crack propagation mechanisms and (screw) dislocation glide with DFT accuracy. We then perform molecular static and dynamics simulations using the open-source code LAMMPS [2]. The simulations reveal the interplay between crack propagation and local hydrogen trapping. Dislocation plasticity in presence of H is investigated by modelling edge dislocations and using an empirical EAM potential [4], which captures the correct lattice parameter, elastic constant, Fe-H interaction and core structure. The influence of dislocation line length, varying distribution, and concentration of H atoms around the dislocation core is systematically investigated.

A significant increase in the Peierls stress is observed at low temperatures due to the dislocation pinning originating from the strong interaction (~ 0.4 eV) of H atoms at the dislocation core. This interaction energy leads to dislocation core saturation up to room temperature for lattice concentrations greater than 0.1 at.%. At finite temperatures up to T=300K, three different regimes, i.e., pinning, solute drag, and unpinning governed by the applied stress and temperature are observed. In the solute drag regime at T=300K, nearly three orders of magnitude reduction in dislocation mobility is observed as compared to the pure Fe case.

This observation of lower dislocation mobility in presence of H contradicts the existing notion that H enhances plasticity by increasing dislocation mobility. Instead, the reduced mobility of dislocations around pre-existing cracks can favour embrittlement over ductile fracture.

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Sequences of Fast and Slow Ruptures on a Frictional Interface in an Elasto-plastic Solid: Application to Earthquake Modeling

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Earthquakes are among the most damaging natural hazards. Our current understanding of earthquakes suggest that they nucleate as instabilities under slow tectonic loading and propagate as shear fractures, mostly at sub-Rayleigh speeds but occasionally as supershear cracks. During an earthquake, the change in the strain energy from the bulk is transformed in fracture energy to facilitate the breakdown processes, heat due to frictional dissipation, radiated energy in the far-field, and inelastic dissipation in the near-field.

While significant progress has been made in understanding earthquake source processes in linear elastic domains, the effect of more realistic inelastic rheologies including plasticity is poorly understood. Here, we simulate the co-evolution of shear fractures on pre-existing fault surfaces and bulk inelastic deformation through modeling a sequence of (fast) earthquakes and (slow) aseismic slip of a 2D rate-and-state frictional interface embedded in a full-space elastic-plastic bulk. We use a computationally efficient hybrid finite element spectral boundary integral scheme that relies on domain decomposition in space and extreme adaptive stepping in time. The hybrid computational scheme enables exact near-field truncation of the elastodynamic field allowing us to use high resolution finite element discretization in a narrow region surrounding the fault zone that encompasses the potential plastic deformation. Wave propagation and long range static stress transfer in the exterior half spaces are handled using the spectral boundary integral equation. The adaptive time stepping is based on the maximum velocity jump across the fault surface. The resulting time step varies from milliseconds to days enabling the simulation of both slow deformation and fast dynamic ruptures over multiple earthquake cycles.

We show that off-fault plasticity may lead to partial ruptures as well as temporal clustering of seismic events. Furthermore, the interaction of fault slip and off-fault plasticity results in pockets of slip deficit signaling that part of the permanent deformation is accommodated in the bulk as inelastic strain. This is different from purely elastic case where all the inelastic deformation is localized as slip on the fault surface. While the energy dissipated through plastic deformation remains a small fraction of the total energy budget, if the yield stress is high enough compared to the fault reference frictional strength, its impact on the source characteristics is disproportionally large through the redistribution of stresses and viscous relaxation. However, if the yield stress of the bulk approaches the frictional strength of the fault, new family of rupture patterns emerge characterized by significant energy dissipation in the bulk and localized slow or creeping ruptures on the fault with no inertia effects Our results emphasize the critical role of bulk strength in controlling multi scale earthquake dynamics and suggest a new mechanism of dynamic heterogeneity in earthquake physics that may have important implications on earthquake size distribution and energy budget. Our findings may also shed light on the dynamics of other systems with similar co-evolutionary processes such as grain boundaries in crystalline structures.

Configurational Peridynamics

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Deformational and configurational mechanics provides information about the motion of a continuum body. Deformational mechanics is concerned with the response of a mechanical system to externally applied loading. These 'standard' forces are associated with the motion of material points in space. Configurational mechanics on the other hand studies forces responsible for the evolution of material structure, i.e., configurational forces are associated with displacements of particles with respect to the surrounding material. As a result configurational forces provides insight into the role of defects and singularities such as dislocations, inhomogeneities, inclusions, interfaces and cracks on material behavior, see e.g. [1, 2].

Peridynamics (PD) is a non-local continuum mechanics theory established by Stewart Silling [3]. PD was originally developed to overcome challenges encountered in the classical continuum mechanics formulation when discontinuities such as cracks are present. It has been extensively used to model damage and fracture. This is done using an additional constitutive equation that prescribes the interaction forces between neighbouring material points based on the distance between them. This allows the interaction forces to fade and vanishes as the distance between the points increase.

Configurational PD has the potential to offer an energy driven model for damage and fracture that is non-local and fully non-linear. Configurational PD offers a framework wherein the key characteristics of initiation and propagation of fracture can be captured; i.e., changes in the topology associated with the geometry of the body accompanying crack initiation and dissipation inside the body associated with propagation of the crack.

This contribution will present the theoretical framework for configurational peridynamics along with computational examples. These examples illustrate the potential of the formulation and highlight key differences from local configurational mechanics.

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Hierarchical Microstructure Controls Interface Failure Patterns

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Hierarchical materials are complex, multi-scale systems where structural patterns are repeated across scales in a self-similar fashion. Hierarchical microstructural patterns are often credited as determinant factors in the high fault tolerance of biological and bio-inspired materials. In problems of interface failure an example is the Geckos paw, where hierarchically structured fibers are believed to play a role in its strong adhesion behavior, which is maintained over many cycles of attachment and detachment [1]. In the broader context of fracture mechanics, the fact that hierarchical organization is integral to enhanced fracture toughness is now widely accepted [2].

Modeling hierarchical structures is naturally a multiscale problem, where stress redistribution and crack propagation must be accounted for at the different microstructural levels. To address this problem, discrete hierarchical lattice/network models have been used in recent years, where the network constituents are elastic load-carrying elements, subject to a failure criterion. Models of this type have helped show the mechanisms by which hierarchical materials induce localized patterns of stress redistribution, which result in the arrest of crack propagation, the emergence of diffuse damage, and the increase of fault tolerance. This behavior has been recently confirmed in experiments with hierarchically patterned semibrittle materials [3].

While most of the above results deal with bulk fracture, here we address the problem of interface adhesion and failure/detachment of hierarchical materials in contact with heterogeneous substrates. To this end, we introduce a three-dimensional hierarchical network model, where discrete links/elements fail based on a maximum distortion energy (von Mises) criterion with Weibull distributed thresholds, modeling inhomogeneities in local cohesive and adhesive strengths. Element elasticity is modeled both in terms of the scalar Random Fuse Model and of the tensorial Timoschenko beam theory.

We find that the hierarchical structure induces scale invariant detachment patterns, which in the limit of low interface disorder prevent interface failure by crack propagation ("detachment fronts") [4]. In the opposite limit of high interface disorder, hierarchical patterns ensure enhanced work of failure as compared to reference non-hierarchical structures.

Our statistical analysis of fracture surfaces indicates that the hierarchical organization is responsible for a substantial enhancement in the localization of damage near the interface, confirming the hypothesis that similar multi-layer fibrous or porous patterns are essential in the performance of bio-inspired reusable and reversible adhesives. We discuss the origin of this localization phenomenon using concepts of spectral graph theory and multiscaling analysis techniques. While our study of hierarchical fracture and failure is motivated by examples of fibrous materials of biological interest, our results indicate that hierarchical patterns can be useful in engineering scenarios where the focus is on tuning and optimizing adhesion properties.

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Fracture surface topology via Phase field modelling: Statistical aspects

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Fracture, being the most encountered failure mode in design, needs to be prevented. Computational modelling of fracture is an indispensable tool not only to predict the failure of cracked structures; but also, to gain an insight to fracture processes. Linear Elastic Fracture Mechanics (LEFM) has been explained by the pioneer works of Griffith et al [1] and Irwin et al [2]. Still, predictive modelling of fracture patterns in materials and structures poses a significant challenge. Fracture of solids can be numerically modelled using either a discontinuous approach (LEFM, CZM) or a continuous approach (Phase Field Modelling (PFM), Peri-Dynamics). The observation of universal scaling behavior on real fracture surfaces has raised hope for a unified theoretical framework to capture fracture processes in disordered solids. However, such a quantitative understanding of the scaling properties is still missing. Ponson at al [3] showed that most experimental fracture surfaces report persistent fracture profiles with large roughness (Hurst) exponent ($H \geq 0.5$) characterized by failure due to damage coalescence, whereas anti-persistence ($H \leq 0.5$) is predicted by LEFM and characterized as brittle fracture processes. H is also claimed to be universal, irrespective of loading and crack pattern.

The present work attempts verification of the above claim of universality computationally using PFM. A two-dimensional Single Edge Notched Tension (SENT) Steel specimen with an initial notch of size equal to half of the specimen width was considered. The plate was subjected to linearly increasing displacements at the top and bottom edges. A honeycomb grain structure with weaker grain boundaries succeeds the notch. Rate independent variational PFM approach similar to the work of Miehe et al [4] has been adopted. We attempt to compare H values for different cases of constant and random grain boundary fracture toughness.

It is observed that H indeed depends on the typical length scale for roughness measurements. Brittle fracture patterns tend to vary from small scale persistence to large scale anti-persistence, whereas the situation is reversed for fracture patterns due to damage coalescence. To support these results, a thorough study of three real fracture surfaces of different materials has been performed and similar trends have been observed.

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Comparison of Irreversibility Strategies in Phase-Field Fracture Simulations

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The phase-field fracture model is extensively used for the simulation of crack propagation in various materials. Within the phase-field model the discrete crack is approximated by a smeared function, the phase-field function. For proper simulation results especially in cyclic loading the treatment of the irreversibility condition $\dot{z} < 0$ is crucial. This physical condition, in which the material is not allowed to heal, can be handled by various methods. The most common choice here is the history-field approach by Miehe et al. [1]. Here, the tensile strain energy Ψ^+ in the crack driving force Y is substituted by the history function $\mathcal{H}^n$ - the maximum tensile strain energy of all previous time steps. However, this strategy requires small time step sizes to capture the crack initiation point, and thus simulations might become computationally expensive. Since phase-field fracture simulations are already computationally expensive, especially for complex structures, adequate improvements should be employed. Besides different strategies of adaptive spatial refinement [5] or adaptive temporal refinement, the choice of maintaining irreversibility can also be considered.

In this presentation, we would like to adresse the comparison of different irreversibility strategies according to the correctness of the simulations and their performance. Common irreversibility strategies are the History previous approach, the History current approach, the Damage formulation [2], the Dirichlet-type approach [3], and the penalization approach [4]. For the History current approach the history value $\mathcal{H}^{n+1}$ is computed as the maximum tensile strain energy up to the current time step. Furthermore, in the staggered solution scheme, the displacement equations are solved before the phase-field equations. In the Damage formulation, the irreversibility condition is checked for each degree of freedom after the phase-field equations have been solved. If the irreversibility condition is violated, the nodal phase-field value is changed to its value of the previous time step and constrained in the next time step. For the Dirichlet-type approach, the phase-field variable is fixed to the broken state $z = 0$ if the phase-field variable falls below a given threshold and is constrained from there on. Since the phase-field solution is actively changed within the last two approaches the solution is not in an equilibrium state anymore. Thus a combined convergence check is necessary followed by an equilibration step in case of non-convergence. A suitable limit of the number of outer loops for the combined convergence check is necessary. In the penalization approach, the phase-field equations are extended by adding a penalty term to the energy functional, resulting in an equality to be solved. This term vanishes if the irreversibility condition is not violated.

For the comparison, a cyclic shear test is conducted where each strategy is tested for proper physical simulation results and performance.

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Combining Damage and Fracture Mechanics for the identification of crack propagation parameters

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This presentation deals with accurate identifications of the crack tip position and fracture energy of cracked media. To model fracture or damage, a phase-field model was employed [6, 7] based on the variational formulation of Bourdin et al. [1]. The governing approach used herein was described in detail in Ref. [8], and the corresponding implementation was based on so-called pfm-cracks [4]. This framework allows for parallel computations and mesh refinement with both uniform and locally adapted meshes. Consequently, the phase-field internal length scale can be easily adapted.

A crack opening displacement-controlled virtual test on a decimetric beam representative of mortar was studied. The material had a non-negligible fracture process zone size (of the order of one centimeter). This means that the crack tip position cannot be precisely determined. In damage mechanics or regularized fracture using phase-field (or peridynamics) [2], the crack tip is usually approximated by a smoothed indicator variable. This is a major difference for this type of model compared to fracture mechanics solutions that explicitly deal with (discontinuous) cracks.

The main objective of this study was to combine phase-field with fracture mechanics models to extract the crack tip position from the simulations in addition to the fracture energy and process zone size. The analysis was inspired by the use of Williams' series [9] in integrated Digital Image Correlation [3] and elastoplastic simulations [5]. In the present case, instead of using experimentally measured displacement fields, they resulted from phase-field simulations to determine the amplitudes of each Williams' field via least squares minimization. The proposed approach accounted for various mesh refinements, as well as the analysis of the numerical and identification residuals.

The results allowed us to conclude about the dependence between the phase-field variable at the crack tip and the internal length at any loading step. This conclusion adds more knowledge and accuracy to usual criteria in damage mechanics that approximate the crack tip position for a fixed damage level.

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Towards a proper and efficient continuum constitutive laws of plain and reinforced concrete specimens – a short comparative study

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The presence of cracks in concrete causes very serious difficulties in its precise and physically meaningful mathematical description. Within continuum mechanics there are basically two alternative approaches to handle cracks: as continuous smeared localisation zones or as discrete displacement jumps. Although the latter method describes better macro-cracks, in analysis of larger specimens ("engineering practice") smeared based constitutive laws are widely used. Three main group of models can be distinguished. First are formulated within continuum damage mechanics with isotropic or anisotropic damage variable/variables. In the simplest formulations only one damage variable is defined, while more advanced laws use different measures to independently describe selected phenomena. The second group utilises elasto-plasticity with one or more failure criteria. Finally both approaches can be coupled to take into account both the stiffness degradation and the occurrence of permanent strains. Despite a huge number of existing models, several issues are still open, especially when concrete is subjected to multiaxial stress state.

The paper is a further continuation of previous works [1, 2] where different continuum constitutive laws for concrete were examined to check their ability to simulate the behaviour of plain and reinforced concrete specimens. Here three very sophisticated formulations are analysed. First a model proposed by Červenka and Papanikolaou [3] is chosen in which Menetrey-Willam failure surface in compression was coupled with orthotropic smeared crack approach in tension. The second law used here has been proposed by Grassl and his co-workers [4] and it is based on elasto-plasticity defined in the effective stress space followed by continuum damage mechanics. As a third alternative idea a proposal given by Marzec and Tejchman is analysed [5], which is also based on the same idea as in [4]. As a regularization technique two methods are implemented and examined: fracture energy/crack band approach and an non-local integral theory. The first solution has been originally used in the models formulated in [3, 4], while the second idea was utilised in [5] (and also in [1,2]).

The analysis of all constitutive laws is focused on two aspects: the compatibility of obtained numerical results with experimental outcomes (to be proper) and the identification of the essential features responsible to give opportunity to reduce the complexity of the formulations (to be efficient). The performed analyses deal with two dimensional problems. First a thorough "local" (at a material point level) analysis under complex stress state is performed. Then selected benchmarks of plain (e.g. Nooru-Mohamed test) and reinforced concrete specimens (e.g. bending of a RE beam) are executed. Obtained results are analysed and compared with experiments.

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Experimental and numerical investigation of cracking in steel fibre reinforced high performance concrete members

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High performance concrete (HPC) is a quite novel material which has been rapidly developed in the last few decades. It exhibits superior mechanical properties and durability comparing to normal concrete. HPC can achieve also superior tensile performance if strong fibres (steel or carbon) are implemented in the matrix.

The motivation for this study is a new material design for wave energy convertor (WEC) floater hull, which requires exceptional performance in harsh marine environment under extreme weather conditions over the course of the service-life of minimum 25 years [1]. Fibre reinforced concrete (FRC) utilises its highest performance after initial cracking, exhibiting strain-hardening when the cracks bridged by fibres redistribute the stresses over larger volume of concrete and thus increases the load bearing capacity of the element. The post-cracking behaviour depends greatly on the fibres content, type, geometry, strength and stiffness, as well as the bond between the fibres and the concrete material. Moreover, fibres orientation in the concrete volume is of importance and it usually makes FRC an anisotropic material dependent on the casting direction, what is especially important in thin-walled elements, where the element geometry forces fibres alignment in one direction.

To be able to understand the influence of the fibres content and bond behaviour (dependent also on shape) on the overall behaviour of FRC, numerical models can be used. Such simulation tools are currently under intensive development along with the definition of new concrete mixtures and continuous growth of knowledge about its performance. Two main approaches to describe the behaviour of fibre reinforced concrete can be identified. In the first method fibre reinforced concrete is analysed as a homogeneous material, so the presence of fibres is taken into account only indirectly (so called 'continuous type') e.g. [2]. The alternative idea is based on an explicit definition of fibres distribution (so called 'discrete type') e.g. [3]. Several model were defined base on this approach. In these formulations the slip between fibres can be either neglected (perfect bond), explicitly modelled or it can be indirectly taken into account via the modification of the constitutive relations for fibres.

The goal of the paper is to introduce the numerical tool in order to investigate the behaviour FRC members. The idea is to use the Finite Element Analysis and mesoscale modelling approach to determine the properties of FRC. The main concept of presented approach is to assume the fully 3D modelling with taking into account explicitly the distribution and orientation of the steel fibres. Different approaches in order to simulate the interaction between fibres and concrete are investigated: accurate methods with an explicitly defined contact law and a simplified (indirect) ones assuming only modifications of the material description for steel fibres. Alternatively, a homogeneous law with trilinear softening curve is used. As a benchmark, results obtained from experimental campaign on beams and panels made from high-performance concrete with steel fibres of different sizes and dosages are taken. Results of numerical simulations (especially force-displacement curves) are directly compared with experimental outcomes in order to validate and calibrate FE-model.

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Modeling Fracture Behavior of Brazilian Splitting Tests Using Micromechanics-based Variational Phase-field Method

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The Brazilian splitting test is an indirect method for measuring the tensile strength of brittle materials, assuming that failure occurs at the center of the disc, where stress is theoretically equal to the ultimate tensile strength. However, the difficulties in determining the crack initiation point in experimental setups has led to debate over the validity of the measured tensile strength [3]. Studies show that failure is not always modulated by mode I fracture energy in the Brazilian splitting test. Material properties (compressive over tensile strength ratio, inhomogeneity, friction angle) or boundary conditions can change the fracture mode from mode I (tensile) to mode II (shear) [2, 3]. This has been studied using the micromechanics-based phase-field model. Micromechanics-based phase-field modeling is an approach used to study the behavior of quasi-brittle materials like mortar and concrete. The aim of this model is to connect field variables at the macroscale with physical dissipative mechanisms at the microcrack level. The model distinguishes between close and open microcracks to capture different fracture modes naturally, without implementing heuristic energy decompositions [1]. This feature is used to simulate the fracture behavior of mortars in the Brazilian splitting test.

The viscoplastic regularization is introduced to the model in order to overcome numerical issues caused by stress concentration near applied loads. The response of a single volume element under homogeneous strain field is studied to explain the effect of confining pressure in the Brazilian splitting test and compared to the analytical solution. Different loading conditions were applied to the volume element to identify different failure modes, utilizing the model's main feature of distinguishing between fracture modes. Results indicated that under biaxial confining pressure and axial tension, the element may experience a tensile or shear fracture depending on the level of biaxial compression, which explains the reason for the observed mode II fracture in the simulation. Additionally, Brazilian splitting tests are conducted using Digital Image Correlation technique to capture the strain field and calibrate the numerical parameters of the model. The model is next validated using experimental data from the work of Deresse et el. [4] and calibrated parameters are used to predict the failure behavior of other samples with the same material but different geometry and boundary conditions. Results show that the numerical failure prediction is consistent with the experiment, confirming the validity and reliability of the simulation model and its ability to predict material behavior and fracture modes under specific loading conditions.

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Z-cracks – Industrial validation of a 3D fracture mechanics simulation software

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The development of ultra-efficient and highly optimized aircraft engines for next-generation commercial jets plays a crucial role to slash greenhouse gas emissions from aviation by 2050. Disruptive technologies and architectures as well as new materials are required to provide the foundation for an upcoming generation of more sustainable engines, thus pushing back the limits of the design processes.

Aircraft engine structures are subjected to cyclic and severe thermomechanical environments. Among the certification specifications defined by aviation regulatory authorities, the damage tolerance of engine critical parts is of particular concern regarding flight safety [1]. Aircraft engine manufacturers must ensure the structural integrity of their products assuming the presence of initial flaws in critical components. The potential for failure from material, manufacturing and service-induced anomalies within the approved lifetime must therefore be assessed to prevent any hazardous engine effects.

The prediction of fatigue crack growth is a major research topic and requires handling complex 3D problems through the development of efficient and reliable methodologies. During the last decades, predictions of crack paths and propagation kinetics have been performed using either analytical approaches, relying on libraries of stress intensity factor solutions [2], or numerical ones, taking advantage of the flexibility of computational techniques such as the finite element method [3].

The present work is dedicated to the industrial validation of Z-cracks, a state-of-the-art 3D fracture mechanics simulation software based on explicit and adaptive remeshing techniques [4, 5]. The aim is to describe how such a tool is validated in an industrial context to be further integrated in the design process of aircraft engine structures. By extending the classical definition of Technology Readiness Levels (TRLs), a maturity assessment framework consisting in three use case bases is proposed. First, a functional validation base is defined. The standard quantities of interest of fracture mechanics (*e.g.*, energy release rate, stress intensity factors, bifurcation angle) are computed for a set of elementary cases and compared to analytical solutions. Then, a technological validation base encompassing specimens representative of engine critical zones is outlined. Fatigue crack growth simulations are performed and compared to experimental data (*e.g.*, crack length, number of cycles, crack front shape) gathered on several test campaigns. Finally, industrial cases are considered and comparisons between experimental and numerical results are carried out based on lessons learnt from real engine parts. The proposed framework is thus generic and offers an efficient step-by-step approach to validate a given software by covering a wide range of applications with increasing complexity.

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Minisymposium DDF:

Data, damage and fracture

Organized by O. Allix and P. Carrara

Experimental mechanics and fracture: Toward a big data approach?

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One of the main sources of data in experimental solid mechanics comes from the use of digital images and their registration via correlation techniques. Thanks to such measurements, one may state that experimental mechanics has entered the big-data world [1]. Adapted inverse techniques have been proposed to use such data for constitutive model identification [2]. In Ref. [3], the authors have inferred failure initiation criteria with an interior approach. It consisted in analyzing all the strain-stress pairs that did not not generate failure. For a ductile Ti 6-4 alloy at a mesoscopic level, its was shown that Rankine's criterion was well suited while criteria based on other quantities failed to give consistent results for both thin and thick notched samples submitted to tension.

The new possibilities associated with data-driven approaches, machine learning and artificial intelligence invite us to question and revisit the exploitation of data generated in such tests. Many data generated in mechanical tests are often not or not completely exploited. For example one may think of:

- all the set of images (partially exploited in the present case)
- micrographs of the surface of failure (not exploited yet)
- the shape of the broken specimen (not exploited).

In the presentation, we will first discuss the experiment itself [4, 3] before opening discussions on the type of approaches that could be used to merge all these different types of data. Another part of the discussion will concern the extension to the case of rupture of the work concerning the learning of behavioral laws [5]. A fundamental question concerns the introduction of physical knowledge within learning processes, which could / should be performed when dealing with failure.

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Multiscale and multiview DIC for damage detection and quantification

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Experimental data on damage and fracture initiation and growth play an important role for developing and/or validating numerical models. Digital Image Correlation techniques (DIC) [1, 2] provide useful information by measuring full displacement fields and identification means of model parameters, as well as quantitative validation procedures of structural models [3]. When dealing with large-scale structures, using several cameras provides very useful data in different parts of interest with different resolutions and uncertainties. However, the combination of multiscale and multiview approaches remains a delicate task. In particular, it is necessary to couple the scales in the most integrated way possible [4] in order to minimize measurement uncertainties and create seamless procedures between tests and simulations for the characterization and prediction of damage in structures.

A multiscale and multiview DIC (MM-DIC) framework has been developed and validated by performing a three-point flexural test on a notched concrete beam using three different cameras. As opposed to a regular DIC with a single camera, the multiview system required additional steps to be able to express the measurement results in a unique frame, which was that of the virtual FE mesh. Calibration was a necessary step since multiple cameras with different resolutions were used to monitor different zones of the sample surface. A backtracking procedure was also performed to properly overlay the images and the corresponding part of the master mesh and the scale factor between camera frames and the FE model. The computation of the Hessian matrices related to each camera and assembling the global one was required for the MM DIC to be performed. Then, the second member vectors related to each camera and for each iteration were computed and assembled. The nodal displacement increments of each image state were then updated and the measured displacement fields were obtained.

For any measurement to be meaningful, uncertainty quantification is necessary [2]. In the present case, the acquisition noise that affected each camera was analyzed by performing a DIC analysis on sequences of reference images with both mono-camera and MM approaches. Mono-scale analyses were also run and the resulting displacement fields were projected onto the unique global mesh and compared to those measured with MM-DIC. MM-DIC enabled the measurement uncertainties to be reduced, also led to lower registration residuals, thus providing more trustworthy displacement fields for the analysis of damage via crack opening displacement fields.

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Modeling the cracking behavior of concrete at the mesoscale

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Crack nucleation and propagation in composite materials like concrete is largely influenced by their mesostructural arrangement. It is nowadays widely accepted that a substantial advancement in understanding their behavior can be gained by modeling explicitly their mesostructure, i.e. by resolving the heterogeneities within the matrix. To obtain realistic 3D geometries an increasingly adopted technique is X-ray computed tomography (CT) [1], which has recently seen great improvements in terms of both spatial and temporal resolution. This technique delivers a large amount of data not only regarding the real mesoscopic arrangement of the phases but also about the crack onset and 3D complex propagation pattern during a mechanical test. The latter information can be obtained from in-situ testing, i.e. by taking several CT images of a sample at different stages of a mechanical test, and from their analysis using Digital Volume Correlation (DVC) to measure the 3D displacement field [4].

The phase-field approach to brittle fracture [2] is a flexible model able to reproduce a broad range of fracture processes including crack nucleation, propagation, branching and merging without introducing ad-hoc criteria. This approach regularizes a sharp crack through the introduction of a phase-field parameter that smoothly varies between 0 (sound material) and 1 (completely cracked) over a support whose width is governed by a small length scale parameter.

The aim of this work is to calibrate and validate the phase field model for brittle fracture of the cement mortar to reproduce the cracking behavior of real concrete at the mesoscale, namely, where an appropriate fraction of aggregates and pores are explicitly resolved. To this end, experimental tests are performed to characterize the elastic and the fracture parameters of both mortar and aggregates. To obtain a validation dataset, a series of in-situ wedge splitting tests [3] is performed on concrete specimens doped with baryte contrast enhancers to enable the automatic segmentation of aggregates and matrix [1]. 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 realistic boundary conditions that can be used as input in the numerical analysis. Also, the adopted procedure provides the 3D evolution of the crack pattern and a full-field displacement dataset. Finally, the calibrated model is validated by comparing numerical and experimental results.

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Investigation of the response of masonry arches using data-driven structural analysis

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Masonry arches are efficient load-bearing structures, which distribute applied loads through compression in adjacent masonry stones. The typical mode of failure for masonry arches is the formation of tension hinges in-between the masonry stones, activated when the thrust line falls outside the section of the masonry arch [1]. The change of the structural state, from equilibrium to mechanism, can be caused by settlement of supports due to earthquakes, vertical loads due to vehicles, erosion, or ground bearing failure. This hinge mechanism can result in damage and eventually partial or total collapse.

In this article an overall data-driven procedure is proposed, for the investigation of the structural response of masonry arches. The main objective of this study is to use machine learning tools in order to predict the structural response of masonry arches in a computationally efficient framework, see also [2, 3]. Heyman's assumptions are adopted for the material behaviour, incorporating contact-friction laws between adjacent blocks to capture failure. Several non-linear finite element models are developed and solved, to create corresponding databases. This procedure has been implemented using Python, Matlab and commercial finite element software. The proposed scheme can be used to predict the deformed geometry, the collapse mechanism and the ultimate, failure load of masonry arches. Cases studies demonstrate the efficiency of the proposed method, by implementing the method to random masonry arch geometries. The method can be extended towards structural health monitoring applications.

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Uncertainty quantification of the reference temperature T_0 of Reactor Pressure Vessel steel with experimental and numerical computation of fracture toughness tests

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Nuclear plant life extension requires accurate evaluation of the embrittlement of reactor pressure vessel (RPV) steels caused by neutron irradiation. This irradiation induces a shift towards higher temperatures of the ductile-to-brittle transition range. To predict this shift, pre-cracked Compact Tension (CT) specimens - made of representative RPV steel - are used in irradiation surveillance programs to perform fracture toughness tests. These data allow the application of the Master Curve methodology from ASTM E1921 standard [1], which describes the evolution and scatter of fracture toughness depending on the material temperature. The Master Curve enables the determination of the reference temperature, T_0, representing the ductile-to-brittle transition temperature.

However, results from toughness test programs reveal many uncertainties in the evaluation of T_0. Firstly these uncertainties are related to the material variabilities, such as the inherent scatter of fracture toughness and its dependency on temperature, which generate different T_0 values from one test program to another. Because of the limited amount of material available, especially in the irradiated state, the number of tests is restricted, which amplifies deviations in T_0 values. To perform further tests with remnant material, we use mini-CT specimens. Nevertheless, geometric variabilities such as the size of the CT specimen, machining defects and the length and shape of the pre-crack affect the results of T_0.

In order to enhance the robustness of fracture toughness evaluation, we propose to quantify the influence of the uncertainties of T_0 mentioned above by identifying their effects. To do so, we use experimental data and we develop numerical models to perform statistical analyses and sensitivity analyses using machine learning methods. Firstly, a finite element code (FEC) simulates tensile tests on CT specimens at a given temperature. The results are post-processed in a stochastic brittle fracture model (Beremin), providing the probability of failure of the specimen, P_f, according to the measured stress intensity factor K_J. By interpolating these data, our stochastic model allows us to emulate any number of fracture toughness tests, plot the Master Curve and evaluate T_0. Based on this global model, we carry out statistical analyses that enable us to quantify the effects on T_0 of the number of tests, the test temperature, and the specimen size. Then, we apply sensitivity analyses such as Sobol's method to identify the geometric and material parameters that have the most influence on T_0. In particularly, we use crack front values from the EuroDataSet database [2] to develop a Karhunen–Loève model that generates stochastic crack fronts in our FEC. Thus, we quantify the effect of crack front on T_0, and we illustrate the most influential modes of curvatures. These results complete the conclusions from a similar study by Lindqvist et al [3], with this time large data sets and varying crack front curvatures.

These results contribute to developing more cost-effective and optimized test methods to estimate T_0 of RPV steels. However, as our FEC is costly to evaluate, we are developing a surrogate model to substitute it for ongoing and further work.

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Data-driven-multi-scale modelling of anisotropic fracture-induced damage

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A data-driven approach is proposed to construct anisotropic damage models with a minimal number of internal variables from phase field - crack propagation simulations on Representative Volume Elements (RVEs) of quasi-brittle materials [1]. The approach resorts in particular to a harmonic analysis of damage [2] combined with computational homogenization of linear elastic solids. The orientation distribution functions of two elastic moduli [2] are computed numerically at each loading step of an incremental crack simulation, while accounting for the effects of the nucleation and propagation of micro cracks by the phase field method. Given these two functions, the effective elastic tensor of a material without or with micro cracks is uniquely determined. The expansions into two Fourier series of the relative variations of these two functions related to an undamaged reference state and to a damage state make appear damage internal variables naturally. The number and natures of these variables can be optimized by truncating the Fourier series and using PCA (Principal Component Analysis) according to the degree of approximation desired. Thus, 2D and 3D anisotropic damage models can be constructed without resorting to usual assumptions made in damage mechanics. This construction holds for complex microstructures including image-based ones and for arbitrary loading history. 2D and 3D applications, including matrix-inclusions composites, porous media and architected microstructures are investigated to evaluate the accuracy of the models constructed and to show the potential of the approach proposed for constructing arbitrary anisotropic damage models from RVE simulations.

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Model-Free Data-Driven Fracture Mechanics

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We present a model-free data-driven paradigm for variational brittle fracture mechanics where the fracture-related material modeling assumptions are removed from the formulation, while retaining the epistemic laws of fracture that stem from variational principles [1, 2]. In this approach, the fracture constitutive behavior is encoded exclusively in a discrete material data set, leading thus to a data-driven model-free approach [3]. The proposed approach can be adopted to reproduce different fracture propagation regimes, including quasi-static, rate-dependent and fatigue fracture. We consider approaches based on both local and global stability principles, fulfilling in the former case the Kuhn–Tucker conditions for the energy release rate and, in the latter, the minimization of the total free energy. The data-driven solution of the fracture mechanics problem relies on the definition of a discrete quantity, generally termed distance, which attains its minimum in correspondence of the data point that best fulfills the conditions imposed by the global and local minimization principles, leading to the data-driven counterparts of both variational principles. Furthermore, the solution is constrained so as to fulfill the crack irreversibility condition. In this non-conservative framework, the crack extension plays the role of a history variable and the proposed approach belongs to the class of differential materials [4].

The data-driven solution relying on the global minimization approach is based on the minimization of a generalized distance coinciding with the total free energy computed in correspondence of each material point. For local minimization, two alternative data-driven distances are proposed, one based on the closest-point projection of the material data set onto the (analytically known) energy-release rate function and another based on the Kuhn–Tucker conditions.

The capabilities of the approach are tested on examples with different geometries, using artificially generated material data sets, with or without random noise, which reproduce or randomize Griffith and R-curve type fracture models. Also, a convergence study with respect to the number of points and the noise amplitude of the data set is performed.

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Approximation and definition of state variables for a comprehensive description of damage

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Over the past decades, non-linear models describing damage and fracture of architectured materials have highly progressed taking into account varied scenrios of degradation under complex multi-axial loadings. Many of these models remain expansive to numericaly handle and difficult to understand. In parallel, full-field measurement has brought a large quantity of data similar to the output of finite element results. A challenging task for the researcher is to extract information from that quantity of data. By definition, information is comprehensive in opposition to raw data. The extraction of this information needs a langage support. In a classical framework of physics, it generaly relies on state variables and the associated energetic potentials. In this paper, the automatic definition of state variables in two situations will be presented.

The first situation corresponds to a local case where the objective is to simplify an existing constitutive relation. As an example, an anisotropic damage model developped for military applications (highly loaded) has to be simplified to be used for civil applications (not severly loaded). For that, a subset of loadings is first defined as an approximation range. On this set, the response is computed for the initial model. The result is the evolution of several 4th order tensorial variables related to different crack networks. An approximation of these damage variables is chosen as a radial decomposition as well as a norm to be minimized. This classcial Principal Component Analysis leads to the definition of a simplified damage kinematics. Several choices of approximations and errors will be discussed [1, 2].

The second situation corresponds to a structural case where the objective is to simplify fields. The developped point of view relies on local patterns extraction associated to a PUM/GFEM method. After an introduction of this method with a manually constructed handbook of local function describing the local response of a composite in elasticity [4], an automatic building method is evaluated. It is based on the local extraction of features from global fields using Principal Component Analysis. The associated difficulties are shown. This part will end with the possibility to model some fracture in composite materials at the scale of the fiber using a handbook of crack patterns [3].

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Adaptive and variable model order reduction for damage modelling using explicit time integration

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Finite Element (FE) Analysis is widely used in both academia and industry to analyse large structural models. Recent advances in material architectures and manufacturing techniques have resuled in geometrical features that, whilst improving structural performance, result in a length-scale that is orders of magnitude smaller than a typical structural scale. In FE modelling this require a large number of degrees of freedom and time-steps, in case of dynamic analyses using explicit time integration. This is particularly challenging when modelling the damage behaviour where the computational cost is proportional to the geometrical and material non-linearities. To overcome this computational bottleneck, a reliable Reduced Order Modelling (ROM) method is required.

ROM methods function by substituting the high-dimensional models by an equivalent lower-dimensional model with reduced computational expense to achieve a similar level of numerical accuracy [1]. In many implementations this is achieved by adopting an offline-online approach. This pre-computed reduced-basis approach for online computations with ROM works well for linear problems, but they are not suitable for modelling non-linear responses, such as associated with damage propagation. This is because a local change in stiffness degradation in multi-axial loading requires a large parametric-space for the accurate calculation of reduced-basis functions.

The solution developed in this work is aimed at developing a ROM method in explicit time integration without offline training, while retaining the computational accuracy and achieving efficiency. Unlike conventional ROM methods, the snapshots are collected and the reduced basis is calculated in the online model with minimal inputs from the user. Although ROM reduces model dimension, the calculation of the internal force vector is still required. To overcome this, a hyper-reduction method called Energy Conserving Sampling and Weighting (ECSW) is used [2]. This calculates the hyper-reduced internal force vector by analysing just a few elements with non-negative weights computed online. This serves as an approximation to global internal force vector.

As a result of hyper-reduction, some elements are skipped from the time increment and their history variables are not updated. Although methods such as Gappy Data reconstruction are available, they are often expensive when performed during multiple time increments. A computationally efficient reconstruction is introduced by using mixed-time integration in the current work.

The percentage of ROM in online calculation can be varied depending on the accuracy required. Furthermore, Full Order Modelling (FOM) is performed at regular intervals such that linear momentum balance is achieved between ROM and FOM modelling.

The developed framework is tested by analysing mode-I, mode-II and mixed-mode damage propagation. The results are examined by comparing numerical accuracy and computational efficiency when compared to FOM. This is further extended by analysing different mesh sizes to understand the reduction in the number of operations and overall computational cost.

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Lipschitz regularization for Data Driven Computational Damage Mechanics

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In the Finite Element simulations (FE) of materials that undergo softening, regularization is necessary to make the problem well-posed. The regularization introduces a length scale into the problem whereby the results of the FE simulations become mesh independent [1]. The regularization is typically introduced in many ways - for instance, using the gradient of damage variables, using a non-local strain measure for the computation of damage, using a non-local energy release rate for damage computation, etc. Most of the regularization techniques used in the literature rely upon the introduction of the integral or the gradient of some internal variable.

The Data Driven Computational Mechanics (DDCM) has been introduced to perform (FE) simulations without recourse to the constitutive model to describe the behavior of the material [2]. The stress-strain pairs obtained from experiments or other micro-scale simulations are used as the input to perform the FE simulations thereby bypassing the material model altogether. By minimizing a certain distance functional, the *mechanical* and *material* states are found that satisfy the equilibrium equations as well as describe the material behavior. In practice an alternated minimization scheme is used. Convergence is said to have occurred when the mechanical and material states do not change any more between the iterations. It shall be noted that the internal variables that are typically used to describe the inelastic behavior of the materials are not explicitly introduced in the context of DDCM.

Simulations can be performed using DDCM with the data that reflects the softening behavior of the material, for instance from damage. As already mentioned, the internal variables that are typically used to describe the inelastic behavior of the material are not explicitly introduced in DDCM. Hence, the techniques that regularize the problem using for instance the gradient of damage or computing damage from non-local strain measures cannot be used in this case. The current study introduces a regularization technique using the strain variable, wherein the gradient of strain is bound by a certain value as was done in [3]. In [3], a constitutive model has been used to describe the behavior of the material. The introduction of a bound prevents the strains from localizing within an element (or on sets of measure zero) thereby introducing non-locality and a length scale into the problem. In the 2D setting, the gradient of strain is replaced by an equivalent measure that is objective. The bounds are placed on this equivalent strain gradient measure instead.

This study first discusses and describes the regularization technique in a 1D setting and compares its performance with the strain gradient models. Secondly, it extends the formulation to the 2D setting, where the constraint becomes non-linear. The effectiveness of this formulation will be tested for multiple cases and the results will be compared with that of the regularization techniques in the continuum setting. Overall, this methodology can be seen as a first step towards the introduction of regularization in the context of DDCM to simulate the materials undergoing softening.

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Phase-Field Fracture Modeling using Physics-Informed Deep Learning

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Scientific modeling and computation is increasingly leveraging advances in Deep learning [1]. The developments in deep learning allowing it to utilize the physical principles and not depend only on swathes of data, has contributed to wide scientific interest in it. A range of physics-informed deep learning approaches have been developed to learn the solution field of a partial differential equation governing a physical phenomenon including in mechanics. They hold promise to improve computational efficiency compared to the traditional approaches in modeling.

Phase-field fracture modeling [2, 3] recasts the problem of fracture as a variational problem which completely determines the fracture process including crack nucleation, propagation and bifurcation and obviates the need for ad-hoc conditions. In this approach, a phase field is introduced in the formulation which smears a crack. It is however a nonlocal model which includes a small length scale. Resolving this length scale in computation is expensive. Hence, uncertainty quantification, material parameter identification, design optimization, among others, using this approach become prohibitively expensive. We explore the application of physics-informed deep learning to parametric phase-field fracture modeling to overcome this challenge. We use Deep Ritz method (DRM) [4] in which the solution field is represented by a neural network (NN) and the training of the network proceeds by directly minimizing the variational energy of the system.

We first study crack nucleation in a 1-D homogeneous bar with prescribed end displacements (U_t). We turn U_t as a parameter of the problem. Then U_t and coordinate x are both inputs to a NN and displacement (u) and phase (α) fields are outputs. The complexity of the problem arises from the fact that for small U_t, the strain and phase fields are homogeneous. Above a threshold U_t however, solution bifurcates and the homogeneous solution becomes unstable. Phase field localizes in the stable solution leading to a jump in the energy-U_t curve. An NN finds it difficult to approximate the resulting discontinuity. So, we utilize domain-decomposition [5] along parameter axis and use independent NNs to approximate the solution in each domain. Then the overall NN solution is able to represent the discontinuous solution and it agrees well with the finite element analysis (FEA) solution.

We also study crack propagation in a single edge notched plate under prescribed displacement which is a combination of tension and shear. The presence of multiple energy minima makes it challenging to obtain the correct solution when prescribed displacement is not purely tensile. The details of the models and the challenges in obtaining the correct solution will be discussed.

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Phase-field fracture model solved by a mixed formulation for physics-informed neural networks

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This study investigates employing physics-informed neural networks (PINNs) to solve the phase-field method's coupled partial differential equations (PDEs) in fracture. The phase field damage model shows the great capability to address different fracture phenomena, such as crack nucleation, propagation, and branching through finding the solutions to the displacement and damage field PDEs.
By incorporating physical constraints, including physical laws, and initial and/or boundary conditions into the network's loss function, the neural network is able to obtain the solution to a boundary value problem, see [1]. The earlier works have shown the capability of deep learning tools to predict the crack path in quasi-brittle materials, see [2, 3].
In this work, the standard PINNs approach is extended to the mixed PINN formulation, see [4], to address fracture by solving phase-field fracture PDEs. We explore different neural network architectures and training procedures (coupled or sequential) and examine the impact of various material parameters.
The results demonstrate the superior performance of the mixed PINNs formulation in obtaining a unique solution to the problem with respect to other PINNs methodologies. The latter is shown through different numerical examples in 1-D and 2-D setups for different multi-physical problems, thermo-elasticity, and phase-field fracture. The obtained results from the network are later compared to the results of the finite element method that is utilized to solve the identical boundary value problem. Finally, the computational cost and ideas for generalizing the network's predictions for different boundary value problems are discussed.

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Physically recurrent neural networks for homogenization of path-dependent heterogeneous materials

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Owing to their high flexibility and potential to reduce computational costs, machine learning techniques are increasingly popular in solid mechanics. These tools are particularly appealing in multiscale methods, such as FE^2, where the computational effort can quickly become prohibitive in practical applications. While several works in the literature showcase speed gains and accurate predictions for bulk homogenization in a wide range of behaviors, the use of surrogate models to predict damage constitutive behavior is a far less explored topic. For such applications, some of the critical limitations in conventional surrogate models have only recently started to be unveiled and addressed.

In [1], we incorporate knowledge of classical constitutive modeling into a neural network for the bulk homogenization of path-dependent heterogeneous materials. The idea is to embed the physics-based material models used in the full-order micro-model inside the data-driven model. For that, the macroscopic strain is encoded into a set of strain vectors for fictitious material points that are evaluated by the material models. The resulting stresses are then decoded in a homogenization-like step to obtain the macroscopic stresses. By keeping track of the internal variables of each material point in the layer in which the material models are introduced, the network can capture path-dependency naturally.

In this work, we present our recent efforts in extending that strategy to also account for microscale damage. Here, a modified architecture is required to incorporate the representation of the cohesive-zone model, which is employed to describe the constitutive behavior in the interface elements. In the new setting, in addition to the bulk material points, we include cohesive zone points mapping displacement jumps to tractions.

Finally, we particularize the proposed approach to model the constitutive behavior of a composite representative volume element with an elastoplastic matrix, elastic fibers, and microcracking modeled by interface elements. The performance of the network is assessed in a set of loading cases with both monotonic and non-monotonic loading.

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Minisymposium DF:

Ductile fracture

Organized by P.-O. Bouchard, J. M. A. César de Sá and R. H. J. Peerlings

Convergence of continuum damage for ductile failure processes

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The paper compares two damage evolution models describing the degraded material response coupled to thermal softening for ductile failures. Continuum thermodynamics is used to represent the energy dissipation induced by the effective material response, thermal effects and damage evolution. The continuum damage evolution of Lemaitre type is focusing the degradation of the shear response, eventually leading to ductile shear failure. Here, the main prototype for the effective material is the Johnson-Cook model, accounting for deformation hardening, strain rate hardening and temperature degrading effects. Our incentive is to consider the convergence and stability properties in the FE-application considering both damage rate and gradient dependence in the fracture area production.

In the damage modeling we are concerned with:

1. the energy dissipation rate describing a damage coupled to plasticity driving dissipation to the fracture area production process. A special feature is the damage-driving dissipation rate, allowing for elastic and plastic contributions separated by a damage threshold for accumulation of inelastic damage-driving energy, [1].

2. the description of energy dissipation due to fracture area production, involving area production due to ”nucleation” and ”convection” of damage in the temporal evolution of the damage field [2]. The “gradient” fracture area production effect is obtained due to spatial growth of the damage field.

3. the formulation of a nonlocal condition for the damage threshold defining plasticity driven damage evolution. For isothermal conditions, the examples exhibit mesh convergent behavior when using the nonlocal damage threshold, [3].

In the application to a dynamic split-Hopkinson test and two quasi-static tensile test, the gradient damage model is compared to a corresponding rate dependent local model. It appears that the temporal damage evolution removes the pathological mesh dependence in the isothermal case and has a stable behavior without the additional gradient effect, [1].

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Fracture assessment of DED manufactured FGM system using phase-field ductile fracture approach

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Functionally graded materials (FGMs) are among the advanced materials that can be suitably produced using additive manufacturing (AM) technologies. In particular, stainless steel/Inconel FGM systems are well-suited for underwater and aerospace applications, as they possess a combination of excellent properties including high corrosion resistance and good weldability. Directed energy deposition (DED) is AM-based procedure which can be effectively used to manufacture FGMs. Due to the gradient changes of material properties, FGMs are not susceptible to issues like premature failure caused by stress concentration, which is a common difficulty in laminated composites. However, the failure analysis in FGMs can be significantly challenging due to the fact that the energy required for crack propagation in these materials is non-uniform, leading to intricate and potentially unpredictable crack paths.

The inherent capability of the phase-field method (PFM) in dealing with wide range of fracture scenarios including crack initiation, propagation, merging, and branching, without the need for any additional criteria, has attracted scientists in many engineering fields. In recent studies, for instance in [1,2], the fracture analysis and problem of crack tip mode mixity in FGMs was approached by combining PFM with homogenization techniques to account for the spatial variability of properties.

In the present work, the failure in FGMs and multi-materials are systematically investigated using phase-field approach in ductile fracture. Following the author's previous study in [3], the PFM is integrated with the $J2$ plasticity model to account for the plastic deformations, and a plastic threshold value is incorporated to regularize the material post-critical softening behavior. To consider the spatial variations of the properties, the effective values for fracture and elastoplastic properties are calculated using the rule of mixtures. The mathematical description of the model is thermodynamically-consistent and is implemented using finite element method. The validation of the model is conducted through a combination of the numerical and experimental procedures. The influence of the gradation profile on the crack trajectory and quantitative force diagrams is highlighted. The workability of the numerical model is then evaluated against the experimental test data from miniaturized tensile test specimens excised from FGM block consisting of 316L and IN718 powders.

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Gradient-plasticity vs Gradient-damage for the Modelling and Calibration of Ductile Damage

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Even though damage hides invisibly inside the material, it can notably affect manufacturing processes and the product's lifetime. The modelling and identification of this process-induced damage is conducted by means of a fully coupled plasticity-damage continuum material model at finite strains. For regularisation, we contrast different approaches for gradient-enhancement. This comprises "plasticity – gradient-damage", where the gradient-enhancement is placed on the damage variable, as well as "gradient-plasticity – damage" with a gradient-enhanced plasticity formulation. Further attention is paid to the numerical implementation and identification of the associated internal length.

Based on the gradient-enhancement of the free energy [1], multiple types of localisation, such as damage and softening plasticity, can effectively be eliminated by the introduction of additional internal length scales. Different variables are studied to insert strong non-locality for plasticity and damage. This choice does not only affect the scope of the regularisation [2], but also influences the calibration procedure for the material model. For instance, the gradient-enhancement of the damage variable alters the locally prescribed damage evolution, thus for instance a directly identified failure strain is not accurately reproduced. This can complicate inverse parameter identifications, which are especially tedious when a large number of experiments need to be considered simultaneously, e. g. for coupled stress-state dependent damage models. For damage identification, global force responses together with local deformation measurements are utilised to improve the uniqueness of the optimisation problem, cf. [3].

Experiments and numerical examples, which represent different stress states, demonstrate the regularising capabilities and characteristics of the gradient-plasticity approach and the gradient-damage approach. Moreover, further insights into the regularisation and its requirements are presented, which will become evident in the conducted parameter identification for sheet metal.

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A XFEM-CZM Based Methodology for Finite Strain Ductile Fracture

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Ductile metals and alloys are the most used materials for structural components in the aerospace, naval and automotive industries due to their strength and good formability. In order to determine the residual strength or/and damage tolerance of engineering structures, it is crucial to be able to reproduce qualitatively and quantitatively the consecutive steps leading to ductile fracture [1], namely: void nucleation and growth, void coalescence into thin bands creating meso-cracks and finally macro-cracking. Mesh-dependency of the numerical results is a well-known issue when the standard finite element method is employed together with a constitutive model involving ductile damage induced softening (e.g. GTN model). In the literature there are some regularization methods mainly based on non-local methods [2] that require a fine meshing, thus having a high computational cost if the response of large-dimension structures is investigated.

We present here a three-dimensional numerical methodology implemented in ABAQUS as user finite element (UEL), that phenomenologically accounts for the mechanisms leading to the progressive failure. In order to deal with large elastoplastic deformation, we adopt the Updated Lagrangian formulation. Ductile damage is treated using the standard finite element method (FEM) whereas the localization band and further crack, embedded in the finite element, are treated using the extended finite element method (XFEM). The band is treated as a cohesive crack (cohesive XFEM) and its progressive cohesion loss leads to the ultimate crack (standard XFEM). The passage from standard FEM (diffuse damage) to cohesive XFEM (localization band) is triggered by a phenomenological criterion in terms of critical porosity that leads to the formation of a damage localization band. The cohesive zone model relates the traction force vector with the equivalent relative displacement, with a power law form for the evolution of the damage-like variable. Local stress triaxiality controls the orientation of the localization plane and the transition between Mode I and Mode II is treated with a mode mixicity law. The integration of the XFEM is performed by means of a volume averaging based integration (VAI) method, already implemented by Nikolakopoulos et al. [3], which mitigates the need for the existence of integration points on both sides of the discontinuity. We also adopt the F-bar approach to deal with incompressibility. The unified methodology exhibits no mesh dependency and is capable of fairly reproducing all consecutive failure mechanisms and the rupture surface for large elastoplastic deformation without volumetric locking. Future developments include cohesive zone model improvement and other physics motivated criteria to describe the passage from diffusive damage to localization and from localization to rupture [4].

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Fatigue Final Fracture Predction Considering a Non-Local GTN Damage Model

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The fracture toughness of metallic materials is usually quantified using K_{IC}. Typically, K_{IC} [MPa.m0.5] is measured in high-strength materials, showing a linear-elastic fracture behavior. The fracture toughness of 18Ni maraging steel ranges from 60 to 120 MPa.m$^{0.5}$ depending on the finishing temperature during hot rolling, solution, and aging heat treatments [1]. There is also a sample thickness influence on these properties [2]. Valid plane-strain KIC was successfully determined for 18Ni (300) maraging steel, with a thickness of 18 mm, solution treated at 815 °C, air-cooled, and aged for 3 h at 427 °C, 482 °C, and 533 °C and 100 h at 427 °C [3]. However, aged samples with thicknesses of less than 18 mm do not meet the thickness requirement for a plane-strain state, which is required to determine a critical value according to the E399 ASTM standard [4]. Thick sections are usually needed in tooling applications, but AM stimulated the design of thin-walled parts and structures. Therefore, other alternatives to measure fracture toughness are needed. The E1820 ASTM standard [5] offers two additional parameters to measure the fracture toughness of materials with elastoplastic behavior: the J-integral and crack tip opening displacement (CTOD) methods.

An interesting alternative consists in the use of the Gurson-Tvergaard-Needleman (GTN) damage model to predict the onset of fracture in ductile materials. The research team has experience in the use of this ductile damage model to predict fatigue crack growth [6] through several crack tip parameters (cyclic plastic strain and porous damage at the crack tip, crack closure, etc.).

The objective here is to apply the GTN model to the study of final fracture of the 18Ni (300) maraging steel. A first approach to the problem of final fracture of ductile metals subjected to cyclic loads considered a 6082-T6 aluminium alloy. Accordingly, an integral regularization method was applied to define a non-local GTN model, able to deal with deformation localization and strain softening. The study has been submitted for publication, were the fatigue crack growth and final ductile fracture was successfully predicted considering a node release strategy. In fact, near the material K_{IC} the GTN model triggered successive node releases without further increase in the applied load, indicating the occurrence of final fracture in a previously defined crack path. Despite the success in the prediction of final fracture, the results shown mesh dependence. However, the case of the ductile fracture of a tensile specimen and the fatigue life predictions provided mesh independent results, with the same numeric model. Therefore, the prediction of the crack path will also be studied in order to check if the model becomes capable of predicting the final fracture regardless of the employed mesh.

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Lode angle effects on damage initiation in multiphase alloys

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Ductile fracture of engineering alloys is governed by a process of nucleation, growth and coalescence of microvoids. The process is commonly considered to be driven by (equivalent) plastic straining, with a significant dependence on the stress triaxiality ratio, i.e. the first invariant of the stress tensor over the second invariant of the deviatoric stress tensor. However, experimental studies carried out over the past two decades have shown that for many alloys there is also a significant influence of the third invariant of the deviatoric stress tensor, which is usually characterised via the so-called Lode angle – see e.g. [1].

In single phase materials, the Lode angle dependence has been explained by the anisotropic growth of voids. In our study we consider multiphase microstructures with a significant hardness contrast between the phases. In particular, our interest is in dual phase steels, which typically employ comparatively hard martensite particles as a reinforcement in a softer ferrite matrix. The contrast in properties in such microstructures results in strongly heterogeneous microscale stress and strain distributions. The main questions which we aim to address are (i) how this heterogeneity influences the dependence of deformability on the Lode angle (or, more generally, on the stress state) and (ii) whether it might in itself introduce a macroscale Lode angle dependence, even if the microscale constituent phases were Lode angle independent.

To answer these questions, we adopt a highly idealised microstructural model of a two-phase material which proved to be a highly effective vehicle for systematic study in earlier work [2, 3]. It consists of an ensemble of three-dimensional periodic cells containing cube-shaped grains which are randomly assigned the properties of the hard and soft phase according to pre-set volume fractions. Both phases are modelled as isotropic and elasto-viscoplastic. Their failure is characterised by the Johnson–Cook damage criterion, based on the grain averaged stress and strain evolution only. This criterion in its original form is Lode angle independent; however, we also consider a Lode angle dependent extension [4]. Each realisation of the random microstructure, i.e. each periodic cell, is subjected to a range of macroscopic (i.e. average) strain paths which induce different Lode angles until failure of the microstructure is predicted. The effect of stress triaxiality is also probed by superimposing a hydrostatic stress in evaluating the damage criterion.

The simulation results show a pronounced effect of the applied Lode angle on the predicted fracture strain, even for the, Lode angle independent, conventional Johnson–Cook criterion. The effect is consistent with experimental observations. Careful statistical analysis reveals that the macroscopic Lode angle dependence stems from its influence on the local stress triaxiality in damage-sensitive features ('hot spots') in the microstructure.

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Minisymposium DFMS:

Dynamic fracture of materials and structures

Organized by I. Kožar and J. Ožbolt

Wave propagation in damaged ceramics

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Ceramics are used as a light-shielding material. When a projectile penetrates a ceramics target very complex phenomena (such as fragmentation, and pulverization) take place. One of the still misunderstood steps remains the behavior of ceramics just after fragmentation, i.e., the interaction between the projectile and the micro-cracked target and the wave propagation in damaged ceramics.

Two different types of mechanical models to describe damage in ceramics are considered. The first one is a micro-mechanics based damage model [1] where damage is introduced through a physical parameter. During the damage process the mechanical model loses its isotropy and its homogeneity but the geometric homogeneity is preserved. In the second one damage is introduced by the presence of micro-cracks in an isotropic and homogeneous elastic solid [2]. This geometric heterogeneity induces a loss of isotropy and of homogeneity. Both models take into account the physical reality, where geometric and material heterogeneities are present.

For both models we have used a discontinuous Galerkin (DG) numerical scheme, which ensures an efficient parallelization, with a leapfrog scheme for the time discretization and a Godunov-type choice of the flux. In the second model the main focus lies on the contact conditions at crack surfaces (including crack opening and closure and stick-and-slip with Coulomb friction). Here the interfacial numerical Godunov type flux is obtained by solving a non-linear and non-smooth system associated to the boundary conditions.

We have done some specific numerical simulations on wave propagation in a damaged ceramics using both models. The geometry and the boundary conditions of the numerical simulations were chosen to correspond to some experimental settings (see [3, 4]). The first one corresponds to a loading-unloading shock experiment using a gas launcher while the second corresponds to a two-step experiment: the pre-fragmentation of the ceramics using an electrical generator of intense pressure followed by a simple shock experiment on the same gas launcher. The idea of this second test is to create cracks inside the material, without destroying the studied sample. Thus, the ceramic can be recovered for another test (as a plate impact test on a gas launcher). The two models are compared against available experimental data.

Concerning the cracks distribution, we have considered two cases, also inspired from the experimental design. The first one concerns a plane wave acting on region with a circular micro-crack distribution while the second one includes a circular wave acting to a region with parallel micro-cracks. Finally, some other numerical experiments concern architected meta-materials, designed to blast energy dissipation, with a hexagonal distribution of the micro-cracks.

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HVEV: A nonlinear viscoelastic model applied to energetic materials

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In the context of the design of solid propellant, it has been noted that there were significant discrepancies between the predictions of the calculation and the experimental results on models and real objects.

These discrepancies are harmful during the design phases because they prevent from imagining and accessing the most complex geometries with high loading rates.

In order to overcome this issue, a new material model has been built: HVEV.

This model is based on two main elements, on the one hand, the generalized Maxwell's viscoelasticity allowing to mimic the behaviour of our materials at different loading regimes and on the other hand, a damage kinetic based on the principle of equivalent stress [1].

An example taken to verify the relevance of this approach concerns one of the most critical phases of life, the thermal shrinkage and shows a good adequacy of the model with the experimental results as much on the temperatures of appearance as on the position of the cracks in the propellant load.

This behaviour law has been extend to composite explosive with dynamic simulation software (LSDYNA) throw user material law. This implementation allow to predict damage of these materials under vulnerability test.

Tests with drop hammer and split hopkinson pressure bar, shows à dependency of the burn rate with the speed of the hammer and the pressure of the shock wave for non-initiated materials. This increased burn rate is the consequence of damage in the material [2].
Damage variable, micro-fracture and burn rate are linked with empirical experiment in manometric bomb on post-mortem samples.

This progress allow the possibility to simulate coupled simulation, mechanics and combustion, to take into account damage in the reaction speed of the combustion.

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Shock and Impact Response of Glass Reinforced Plastics

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This presentation discusses the application of a hyperelastic continuum damage mechanics (CDM) based constitutive equations, derived from a Helmholtz free energy relationship, to describe the response of fiber composites under shock loading conditions. The energy terms are divided into: shear and bulk deformation of the matrix material, and different fiber systems under both shear and tension.

The CDM model [1] describes various damage modes in a layered woven/planar glass fiber reinforced plastics (GRP). The damage modes are: matrix shear cracking and volume expansion under compressive loading conditions, delamination, fiber breaking under tension and fiber debonding due to bucking of the fiber under compression. The volume increase under compression is modeled using an empirical relationship that captures the effects of wing crack mechanisms based splitting / faulting type mode 1 fracture in the brittle matrix material.

Tsai et al., [2] conducted shock wave propagation experiments to study the compressive failure of GRP and whose data is used extensively in this study. The effects of various damage modes on the free surface velocity profiles in a plate impact shock wave propagation test are studied through ALE 3D finite element code [2] simulations. The comparisons between VISAR data and computed free surface velocity profiles aided the calibration of parameters for the strain-based damage initiation and propagation models.

Based on the simulation results, with the absence of any permanent strains, such as the plastic strain, the HEL point is interpreted as the onset of elastic-elastic cracking (EEC) of the matrix materials under compressive loading. The strain-based damage initiation and propagation models have several model parameters. In the simulations, the matrix damage (microcracking of the matrix) emanates from the impact plane and progressively damage the GRP target plate in the plate impact experiments. A number of plate impact configurations with steel or aluminum flyers are simulated at a range of impact velocities varying between 100 and 500 m/s. The simulation showed that the lateral stresses increased to the shock stress level when the ratio of shear and bulk moduli became zero, and thus generating a hydrostatic pressure condition in the GRP. The code results further revealed that the Hugoniot relaxed to the hydrostat by unloading along the degraded moduli, and the longitudinal shock wave speed reduced to bulk wave speed.

This work further examined the possibility of extending the CDM / hyperelasticity model to predict depth of penetration of a projectile into thick target plates at high velocities. The main focus of the ballistic modeling was to develop a better understanding of the penetration resistance due to fiber stretching under radial tension. While the plate impact captured energy dissipation due to matrix cracking and pulverization, the ballistic impact provided an opportunity to validate the generality of the calibrated model parameters through comparison between the depth of penetration measured in ballistic tests and hydrocode simulations.

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Comparison between cohesive elements and the Lip-field approach to fracture in 1D dynamic fragmentation

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The dynamic fragmentation phenomenon is characterized as a fast, explosive, and complex failure of solids when submitted to extreme loads. It involves the initiation, propagation, branching, and merging of cracks, leading to fragment formation. Crack modeling is a key factor in the simulation of this complex crack process and is of interest to engineers and researchers engaged in problems involving hypervelocity impacts. An example is the concern of the aerospace industry with the increasing number of space debris orbiting the Earth, since these objects can collide with satellites, leading to a dynamic fragmentation of important structures.

The Lip-field approach to fracture was introduced in [1] for 1D cases and for 2D in [2]. It was also already extended to 1D dynamics in [3]. It is a diffuse damage approach, similarly to most damage mechanics based models, where the loss of strength, or other mechanical property, is a function of an irreversible scalar field called damage. The Lip-field methodology enforces this damage field to be Lipschitz continuous by solving a an optimization problem subject to a Lipschitz constraint.

In the context of the Finite Element Method (FEM), a popular approach to modeling cracks is the Cohesive Zone Model (CZM). It proposes the insertion of cohesive elements on the facets of finite elements when failure conditions are met. By modifying the mesh, jumps in displacement are admitted into the model, and this enables the evolution of the crack opening based on a cohesive law.

Both methodologies (cohesive elements insertion and diffuse damage models) have benefits and drawbacks. Note that for CZM, cracks can only propagate through paths formed by mesh facets, and hence the usual caveat is a strong mesh dependency. On the other hand, for diffuse damage models, when using FE discretizations, a regularization length is used to avoid the concentration of damage and reduce mesh-dependency. Their leading drawback is a high computational cost. They also lack an explicit crack path definition, which comes naturally when using cohesive elements.

In this study, we compare the CZM and Lip-field by means of fragmentation data (i.e. number and size of fragments), and computational cost, in a 1D dynamic fragmentation of an expanding ring. A comparison between the two approaches was done in [3]. Here, we extend this comparison by considering contact forces occurring between newly created cracked surfaces.

The comparisons made in this study contribute to a better understanding of the benefits and drawbacks of each approaches when analyzing fast and complex facture processes.

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Load rate as a material model parameter

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In the dynamic analysis of materials and structures, the load rate is usually applied after the discretization of the model. As a result, the left and right sides of the equation are treated separately. This can lead to a loss of insight into the structure/ material behaviour or even to incorrect results. In the approach presented, the structure, material, and loading are analysed together as a nonlinear dynamic system. The resulting equations are a system of nonlinear differential algebraic equations (DAE). Thus, the material and loading parameters are coupled and their mutual interaction can be analysed [1].

In previous work, the material model consisted of a series of Maxwell cells [2] or Kelvin cells [3]. The Maxwell model is used to describe fluid materials and the Kelvin model is used to describe solid materials. Here, the Burgers material model is proposed [4] because it can assume the behaviour of either the Maxwell or Kelvin model depending on the parameters. Since the model parameters can be changed during the analysis, it can represent complex phenomena such as solidification or melting, etc.

Dynamic analysis is required to study the rate behaviour of a material. It is possible to simulate a force- or displacement-driven experiment. In the first case we have Neumann boundary conditions and in the second case Dirichlet boundary conditions. We use a displacement controlled model since this provides a unique relationship for our softening material. The sudden loading is simulated with the impact loading, but the periodic loading with different frequencies is also needed to analyse the material response. The amplitudes of the two types of loading are kept equal.

The Burger model is a combination of the basic Maxwell and Kelvin material models in such a way that, given a suitable choice of material parameters, one can obtain either one of the basic models or a combination of them. We could say that the basic models represent the two limits and the model behavior lies somewhere between these two extremes. In each material cell, we have four parameters: the Maxwell elastic modulus and viscous damper, and the Kelvin elastic modulus and viscous damper. The external variable of the cell is its strain/displacement. There are also three internal variables: elastic and viscous strains in the Maxwell part and strain in the Kelvin part of the model. The evolution model of the internal variables is assumed to be nonlinear. For the elastic moduli, we have relationships that are used in the microplane material model. Each material cell can be without (viscous model) or with a mass (dynamic model).

Structural models include a larger number of material cells, limited only by computer capacity. Therefore, methods for automatic generation of DAE need to be developed. In this work, a matrix formulation is used that takes into account the different properties of the Maxwell and Kelvin components of the Burger model. The response of the structure is evaluated using phase diagrams, spectrograms, and power spectral density (PSD) diagrams.

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A new paradigm to study dynamic shear crack propagation and friction evolution

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Experimentally measuring the behavior of dynamic cracks is very elusive due to metrological challenges associated with the high speeds of deformation. Yet, physically based models of dynamic cracks require key inputs from experimental measurements. In this work, we present our novel experimental approach to study dynamic shear cracks and friction evolution in real time, using the digital image correlation (DIC) method.

Characterizing dynamic shear cracks and how friction evolves poses several metrological challenges as it is difficult to measure the full-field velocities and stresses close to the interface during sliding. Our approach is based on digital image correlation combined with ultrahigh-speed photography. To capture the highly transient nature of dynamic cracks we employ frame rates of up to 2 million frames/sec and a highly-tailored analysis [1,2]. Our experimental configuration features two quadrilateral plates in contact over an inclined frictional interface, loaded in shear and compression. The plates are made of a polymer, typically either Homalite-100 or PMMA. Dynamic rupture is initiated by the small pressure discharge due to a thin filament of NiCr placed across the interface.

Our measurements allow us to visualize the full-field behavior of spontaneously evolving dynamic shear cracks and to characterize the patterns of sub-Rayleigh and supershear ruptures with a level of accuracy that, until recently, was only possible to achieve with numerical simulations [2,3]. Our detailed measurements also reveal the highly heterogeneous structure of the strain rates, which has profound effects on the rupture behavior due to the strain-rate dependent nature of the tested polymers [4].

Friction plays a central role in rupture propagation along interfaces and it influences a broad class of issues, including rupture nucleation, propagation, and arrest. We find that friction evolution is consistent with the rate-and-state friction laws combined with flash heating weakening mechanism but not with the widely used slip-weakening laws. Our recent experiments along interfaces enriched with granular materials, reveal an even more complex behavior characterized by intermittent rupture propagation [5]. The shear strength of the compressed granular layers initially increases, inhibiting rupture propagation, but later drops promoting rupture re-nucleation. Our observations of the weakening and strengthening behavior of friction in fine granular materials show the pronounced dependence of their rheology on slip velocity and related processes, such as shear heating, and localization and delocalization of shear.

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Phase-field numerical modelling of crack propagation through a fully-explicit time stepping method

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Dynamic fracture arouses interest in many engineering applications under severe dynamic loading such as earthquakes, crashes, blasts, and other impact conditions. Inertial effects and wave propagation contribute to the crack nucleation process, which propagation often leads to structural failure. These phenomona raise many questions in numerical analysis that leads to the development of various models. Among them, the variational phase-field approach becomes popular for its capacity to represent both crack initiation and propagation through a system of coupled variational equations [1]. Originally developed in quasi-static framework, it was extended to dynamic regime. The time incremental approaches can be treated both with implicit or explicit time integration methods. In the literature, implicit schemes are widely chosen for their stability property. But this advantage comes at a computational cost per iteration since it requires the use of non-linear solvers such as Newton Raphson to operate a convergence process within each time increment. On the opposite, explicit methods avoid iterations as well as the resolution of system of linear equations and convergence problems but their stability has to be ensured by a very small time step. To benefit from the advantages of explicit approaches, some authors have proposed strategies of resolution in which both formulations are integrated with an explicit time integration scheme. Nonetheless, this method rises questions about the adaptation of the damage formulation and an appropriate choice of critical time stepping. The damage equation is naturally stated in a quasi-static formulation, non-suitable for explicit time schemes. Some authors have proposed two alternatives to make it compatible with. The first one considers the Ginzburg Landau evolution to the phase-field equation, introducing a viscous parameter weighted the time derivative of the damage [2]. Whereas the second method uses a hyperbolic PDE, characteristic of a wave propagation equation [3]. Both strategies present a formalism that tends to limit the rate of damage evolution and thus, the crack growth speed. Nonetheless the last strategy improves the time resolution through a $\Delta t_c \propto h_{min}$ compared to $\Delta t_c \propto h_{min}^2$ for the parabolic PDE.

The purpose of this work is to propose an efficient resolution of the coupled variational fracture problem compatible with a full-explicit time integration approach and to transfer the resolution algorithms into an industrial explicit code, EUROPLEXUS. To achieve this goal, we undertake a prototyping phase under the open-source platform *FEniCSx.*[1], coupling with a code generator of laws, *MFront/MGIS.*[2]. This tool allows to gather the material knowledges in a standalone library for future use in different solvers. Currently, the code generator is used to provide fracture behavior laws of tension/compression assymetry, preventing spurious crack closure under compressive loads. The aim is to extend his use to nonlinear material behavior and finally achieve to a full-explicit time integration resolution compatible with nonlinear material.

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Hybrid discontinuous Galerkin/cohesive zone model computational framework for dynamic fracture and fragmentation in geometrically exact slender beams

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Exceptional advances in additive manufacturing have recently enabled the development of architected materials with microstructures engineered to achieve unprecedented combinations of properties. For example, architected materials can be designed for high strength and stiffness, at a relatively low weight, or for maximizing energy absorption or dissipation in extreme events. Canonical examples of such architected materials are truss-based micro- and nanolattices, which consist of beam networks in a lattice-based repeating arrangement that have found applications in ultra-lightweight structures for load-bearing and impact absorption. Recent experimental work has shown promising application of such materials for supersonic impact resilience, surpassing kevlar and steel by an order of magnitude in energy-absorption-to-weight ratio [1].

While architected materials with relatively simple topologies can be analyzed based on fundamental approaches, predicting the response of more complex structures in extreme environments requires advanced computational modeling [2]. In fact, the response of architected materials in extreme environments is governed by various energy absorption and dissipation mechanisms, including buckling, fracture, and fragmentation [1, 3].

In this talk, we present a hybrid discontinuous Galerkin (DG)/cohesive zone model (CZM) computational framework capable of modeling buckling, fracture, and fragmentation in truss-based architected materials when subjected to extreme loading environments. The framework is developed by combining the DG discretization of the geometrically-exact large-deformation Kirchhoff beam formulation and the CZM for fracture. The flux and compatibility terms in the DG beam formulation impose continuity at the interfaces before fracture, while a CZM is used to model the fracture process at the element interfaces. An advantage of this framework is its inherent massive parallel scalability, which was demonstrated both in case of dynamic [4] and quasi-static [5] fracture propagation, thus allowing large scale fracture simulations for realistic applications.

Finally, we present numerical results demonstrating the ability of the hybrid discontinuous Galerkin (DG)/cohesive zone model (CZM) framework to capture the relevant physics in beam-based structures exposed to extreme environments.

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Elasto-plastic-damage model for concrete subjected to high strain rates

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Concrete structures subjected to extreme dynamic events, such as impact and explosion, exhibit failure processes in the form of crushing and spalling which differ significantly from those obtained from statically loaded structures [1]. Numerical modelling of these processes requires constitutive models which can describe the increase in tensile and compressive strength with increasing strain rate. In addition, the models should be robust and be based on as few as possible input parameters, which can be determined easily from experiments.

In the present work, a strain rate dependent damage-plasticity model is proposed for modelling both cracking and crushing, and also the strain rate dependence of these processes. The model is based on the previously developed rate-independent version of CDPM2 [2]. The plasticity model is extended by introducing the plastic strain rate in the yield surface while satisfying the consistency conditions as it was proposed in Drysdale and Zak [3]. The damage part is formulated so that a mesh-independent crack opening response is obtained. The constitutive model is implemented in the finite element software OOFEM [4]. The model of concrete is compared to experimental results for a spalling test reported in Schuler et al. [5] and a splitting test reported in Grote et al. [6]. The model is also compared to an earlier version of an extension of CDPM2 in which the damage part was made dependent on the elastic strain rate [7]. Future work will focus on applying the model to reinforced concrete structures for further validation.

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Rate-dependency influence on limiting crack-tip speeds in dynamic phase-field

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Rate-dependent materials such as viscoelastic polymers are abundantly relevant in engineering and real-life applications. This rate (time) dependency is expected to affect their overall behaviour. Specifically, there's a relevant need for exploring their failure behaviour. Moreover, the phase-field approach to fracture has proven to be a powerful tool for the prediction of crack phenomena.

Within this context, this contribution explores three thermodynamically consistent phase-field formulation for rate-dependent fracture in viscoelastic materials. By means of a numerical study on a Uniform Displacement Strip Benchmark, the formulations and modelling assumptions are compared, and the corresponding limiting crack-tip speeds are discussed.

The first formulation [1] is characterised by the addition to the pseudo-energy functional of the phase-field problem (free energy and fracture dissipation) a contribution which is related to viscous dissipation. The viscous dissipation is assumed to promote fracture. It is based on experimental evidence that shows how the resistance to fracture of many rate-dependent materials decreases as the temperature increases - knowing that viscoelastic dissipation leads to a raise in the temperature of the material. In this formulation, we observe viscoelastic hardening in the wake of the crack.

The second model [2] is characterised by the introduction of a strain-rate dependent toughness g_c. It is based on experimental evidence that indicate a strong relationship between the rate of strains and the material's resistance against fracture. This results in a higher strength for faster loading, which directly translates to a higher toughness g_c. In this formulation, quasi-viscous stresses appear in the damaged region around the crack, and we observe viscoelastic-like hardening at the crack-tip.

Alternatively, in the same spirit, we suggest a damage-rate dependent toughness formulation. Naturally, the toughness g_c would be limited by means of the limited damage-rate (damage-delay-like effect) inherent to the phase-field model. Moreover, no hardening at the crack-tip should be observed.

The numerical study lead on a Uniform Displacement Strip Benchmark shows that the three formulations are indeed able to suppress fracture branching in dynamic fracture. The limiting crack-tip speeds are observed to slightly increase as the branching is suppressed. However, for stronger rate-dependent effects (increased viscosity or rate-dependency of the toughness), the mechanical energy dissipation increases; hence, the available energy to advance the crack decreases, which in its turn, suppresses the branching, but also slowers the crack-tip advancement.

Depending on the specific choice of parameters, our simulations show crack propagations at speeds that exceed the shear-wave speeds. Indeed, these high speeds are attributed to the viscoelastic and viscoelastic-like (strain-rate dependent g_c) stiffening at the crack-tip. This translates to faster running surface waves and enables supersonic wave-speeds; a never-seen-before result in phase-field simulations [3].

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Dynamic rupture and fragmentation of a bar with the Phase-field and Lip-field approach

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This work is about the modelling of rupture and fragmentation with the Phase-field and Lip-field approaches. Phase-field [1] has been widely used to model the failure of material since the last few years. On the other hand, Lip-field was introduced more recently in [2] as a new way to regularize softening material models. It was tested in 1D quasistatic in [2] and 2D quasistatic in [3].

The two approaches share some similarities. They formulate the mechanical problem to be solved as the minimization problem of an incremental potential. The minimization problem is not convex if the displacement and damage fields are considered as unknown at the same time. However, looking for the displacement field for a given damage field is a convex problem, and vice versa. Therefore, the displacement and damage field at each time step are usually obtained by a staggered algorithm, where the displacement field is computed for a fixed damage field, then the damage field is computed for a fixed displacement field. Both Phase-field and Lip-field introduce a characteristic length parameter ℓ_c to avoid mesh dependency, the main difference being how this parameter ℓ_c is introduced. In Phase-field, it is taken into account by a term in the incremental potential which depends on the gradient of the damage variable. On the other hand, with Lip-field, a Lipschitz constraint based on ℓ_c is imposed on the damage field. Another feature of the Lip-field approach is to provide bounds on the domain where the Lipschitz constraint is active, allowing to focus computing efforts on restricted zones.

In [4], the Phase-field incremental potential is obtained by equivalence with a linear cohesive zone model (CZM). A similar process was used in [5] for Lip-field. In the present work, we show that several choices are possible to get this CZM equivalence, but that some of them are numerically better than the others. Then, both Phase-field and Lip-field are applied to 1D dynamic rupture and fragmentation examples. In particular, for the fragmentation example and following the work of [5], computations with randomly distributed material properties are performed to get average fragment sizes and dissipated energies, which are compared to several experimental, analytical and numerical references.

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Dynamic fragmentation using phase-field modeling of fracture

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Dynamic fragmentation is a process during which a material or structure subjected to intense loads fails catastrophically through the initiation, propagation and coalescence of a multitude of cracks. It is a key topic in many fields of engineering, as for instance in aerospace industry, where the impact of space debris with satellites is of great concern. Robust numerical models are direly needed to develop a fundamental understanding of such events, in particular to be able to predict the statistical distributions of fragment sizes, shapes and velocities resulting from such a collision.

A well established way to address this problem is to use FE solid mechanics models coupled with cohesive elements [1]. Cohesive cracks give an explicit representation of crack surfaces and simplify the treatment of contacts between fragments, a crucial factor to predict debris velocities. However, the cohesive approach is known to suffer from mesh dependency, with crack paths that depend on the underlying mesh, resulting in non-robust predictions of fragments shapes.

Phase-field modeling of fracture belongs to another family of methods using diffuse crack approaches and, as opposed to cohesive models, where the fracture paths are not dependent on the underlying mesh. Phase-field has been shown to lead to promising results in many problems, not only in quasi-static but also in dynamics where different mechanisms such as branching can be observed [2]. In addition, the multiplicity of possible crack patterns obtained with phase-field for a single loading case in quasi-static has been discussed in [3] where different simulation outcomes can be associated with probabilities. This study is yet to be extended to dynamic cases where the evolution of statistics on fracture paths with the loading rate can be explored. This stochastic approach is of great interest in the context of dynamic fragmentation to enrich statistical data of fragment sizes and shapes in light of material heterogeneity.

The phase-field approach to fracture, addressing the issue of mesh-dependency, will be examined in fragmentation dynamics and numerical data shall be compared to outcomes of cohesive crack models. Then, adaptations of fragment tracking algorithms to diffuse crack approaches will be discussed. Finally, the sensitivity of debris distributions to small variations in the material parameters or the geometry of the model will be analyzed.

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Limitation of the delay damage model in dynamics

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Prediction of damage of structure is still a great challenge until now, especially for dynamic loading. During these last years, many models were proposed to describe damage in structure for dynamic loading. We can cite the Thick Level set damage model [Moreau2015], phase field damage model [Borden2012] and delay damage model [Allix1997, zghal2020]. In this work, we will focus on the delay damage model for dynamic loading.

The delay damage model was introduced by Allix et Deü [Allix1997] as a model that permits to overcome spurious mesh dependency in failure analysis involving damage and dynamic loading. The damage rate is bounded through a time scale which, combined with the wave speed, introduces implicitly a length scale. In this work, we analyze whether or not the model was keeping its promises on three different loading scenarii. We investigate, so, the delay damage model through numerical experiments on three different loading cases of a bar: a slow loading leading to a dynamic failure, pulses, and impact. We observe and discuss the load level needed for failure (and the dependence of this load level with respect to the loading rate), as well as the dissipation and extent of the fully damaged zone at failure [zghal2020]. Observations lead to the following conclusions:

1. First, the delayed damage model has no regularization effect for a dynamic failure initiated from rest.
2. Second, for pulse loadings, the loading rate has no influence on the minimal load level needed for failure (even though the delayed damage model is a time-dependent model), and beyond this minimal load level for failure, the extent of the fully damage zone rises, proportionally to the length scale.
3. Third, regarding the impact, the velocity needed to reach failure depends only on the time-independent parameters of the models and not the ones linked to the delayed damage.

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Minisymposium DMMF:

Discrete models for material failure

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

Carbonation in bacteria based self-healing cement: A new modelling approach

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Concrete, with its excellent resilience and strength, is an excellent building material. It is also relatively low-cost, easy to make and durable. However, in recent years, the cement industry is concerned about its colossal carbon footprint (8% of global CO_2), mostly due to the cement production itself. More sustainable cements and decarbonisation have been forefront in cement research worldwide.

Development of sustainable cement/concrete demands a fundamental scale understanding of its reactions, microstructure and transport properties. Self-healing in concrete is an interesting property which has a lot of potential. When a crack forms in concrete it lets in atmospheric air and humidity. The CO_2 present reacts with the calcium in the cement paste forming calcium carbonate, which acts as a healing material. This work is an attempt to develop first simulations coupling together the bio, the organic, and the mineral, to optimise the self-healing strategy (concrete composition, environmental conditions etc.) for a given material and exposure conditions.

The models of carbonation in concrete must handle both the chemical reactions involved and mechanical and transport phenomena. Bacterial activity in concrete also demands the understanding of bacterial cell division, growth, and nutrient metabolism. Traditional continuum scale models adopts a heuristic assumptions on reaction rates and creates uncertainty while considering new systems. Hence, we are proposing the development of a chemo-mechanical model which can handle the large number of inputs, processes and materials involved in this process. The method uses Kinetic Monte Carlo (KMC) for mineral dissolution and precipitation, while bacterial growth and metabolism are also resolved via direct integration of their kinetic equations. This is achieved by combining two complex code bases.

1) MASKE, which is a recently developed Kinetic Monte Carlo framework [1], [2] for the chemo-mechanical evolution of mineral microstructures. In MASKE, the system is discretized representing the mineral phases as agglomerates of nanoparticles which interact via effective potentials (energy as a function of distance) whose spatial derivatives are the interaction forces. The particles can dissolve and precipitate via reaction rates obtained from transition state theory (TST). MASKE has been shown effective in modelling mineral dissolution-precipitation for cementitious systems and autogenous healing forming calcium carbonate. The system is coarse grained to micro-scale so that particle sizes are comparable to the microbe size.
2) NUFEB (Newcastle University Frontier in Engineering Biology), which is an open-source tool for 3D individual-based simulation of microbial communities. The tool is built a user package for the molecular dynamic simulator LAMMPS and extended with features for microbial modelling [3]– [5].

In this work we combine these code bases, both based on LAMMPS to model self-healing in cement with bacteria. The results predict for the first time the progress of calcium carbonate precipitation within a crack, along with the evolution of the bacterial colony producing CO_2 and the deterioration of the crack surfaces following the dissolution of calcium hydroxide.

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Crackling noise in a discrete element model of shrinkage induced cracking

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Shrinkage induced cracking of thin material layers attached to a substrate gives rise to spectacular polygonal crack patterns. Examples range from drying lake beds through paint layers in art and industry to the columnar joints formed in cooling volcanic lava [1]. Laboratory experiments with desiccating layers of dense suspensions like coffee, clay, and calcium carbonate [1, 2] on rigid substrates revealed that the emerging crack patterns have a cellular structure with a high degree of isotropy in the crack orientation. Recent experiments have demonstrated that applying mechanical perturbation, e.g. vibration to a dense paste before desiccation sets on, the structure of the emerging crack pattern becomes anisotropic, and its structural features can be tuned by controlling the perturbation. Due to its technological potential for microelectronic manufacturing, it is important to explore the intermittent dynamics of shrinkage induced cracking in the presence and absence of anisotropy, where realistic computer simulations are indispensable.

To investigate shrinkage induced cracking phenomena, recently we have introduced a discrete element model which captures the essential mechanisms of crack nucleation and growth in the shrinking layer attached to a substrate, furthermore, the model allows for a representation of anisotropic material properties with a controllable degree of anisotropy [3]. In the model the layer is discretized in terms of randomly shaped convex polygons, which are coupled by beam elements representing their cohesive contacts. Shrinking of the layer is modelled by gradually reducing the natural length of beams, while adhesion to the substrate is ensured by springs connecting the polygons to the underlying plane. Based on computer simulations of the model, here we investigate the temporal evolution of the accumulation of damage in the shrinking layer.

In particular, we demonstrate that cracking of the shrinking layer proceeds in bursts which are trails of correlated local breakings. Single bursts are characterized by their size, and duration, which both fluctuate in broad ranges due to the inherent disorder of the layer material. Our simulations revealed that the probability distribution of the burst size and duration exhibit power law behaviour with exponents which have a weak dependence on the degree of anisotropy. The size and duration of bursts are correlated since larger bursts typically grow for a longer time, which is expressed by a power law relation of the two quantities.

Most notably, we show that the average temporal profile of cracking bursts has a nearly symmetric parabolic shape, which indicates that burst start slowly then accelerate and stop gradually. Based on a careful numerical analysis we obtained the scaling structure of profiles of different durations and gave a detailed characterization of the form of the scaling function.

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Discrete element modelling of the tensile failure of porous rocks

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Rocks experience complex loading conditions including tension, compression, and shear during their geological history. Deformation is accompanied by the release of elastic energy from micro-cracking events, which can be registered in the form of acoustic waves [1]. Acoustic emissions (AE) form the primary source of information about the microscopic processes of fracturing providing us with valuable data about the temporal and spatial evolution of the ensemble micro-cracks leading to ultimate failure. The acoustic noise generated during the compressive failure of rocks in laboratory experiments has been found to exhibit scale-free statistics similar to earthquakes, which addressed the universality of cracking phenomena across a broad range of length scales. In spite of the intensive research, the effect of the loading conditions on the statistical features of crackling noise generating acoustic emissions has not been fully understood.

Due to the limitations of acoustic emission experiments, computer simulations of realistic models of geomaterials can be used to complete our insight into the deformation and fracture of rocks. In order to understand how the loading condition affects the jerky evolution of the fracture process and the spatial structure of damage in porous rocks, here we use discrete element simulations to analyze the statistical and dynamical features of crackling noise emerging during the tensile failure of a realistic model rock and compare the results to the outcomes of simulations obtained under compressive loading of the same samples [3]. In the model numerical porous rock samples are generated by sedimenting spherical particles with a random radius in a cylindrical container under the action gravity. The center of particles are connected by beam elements which represent the cementation of the material. The cylinder is slowly elongated by moving boundary particle layers at the bottom and at top of cylinder against each other.

We demonstrate that under uniaxial tensile loading the system has a quasi-brittle behaviour where the fluctuating ultimate strength and the strain where cracking sets on are both described by Weibull distributions. Simulations showed that as the sample is elongated fracturing proceeds in bursts of microcracks which have a scale free statistics: the size, duration, and energy released by the avalanche are all power law distributed with a finite size cutoff. Simulations revealed that the beginning of the failure process is dominated by the disordered micro-structure of the material which gives rise to random nucleation all over the sample. Approaching failure, breaking avalanches localize and merge into a sharply defined fracture plane at which the specimen falls apart. We give a quantitative characterization of the fluctuating sharpness, orientation, and position of the fracture plane. The results are compared to the outcomes of the simulations of uniaxial compressive failure of the same specimens [3]. In spite of the strong differences of the spatial structure of damage in the two cases, for the statistics of avalanche quantities the same qualitative trends are obtained and also the value of the exponents fall rather close to each other.

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Laboratory measurements and discrete element method calculations of acoustic emission in concrete beams during fracture

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Fracture is one of the most important and challenging issues in concrete materials. A deep understanding of the damage process (crack creation and development) is necessary for safety reasons. Especially, the early prediction of micro-cracks with non-destructive methods is important, nowadays. In this article, the acoustic emission (AE) technique was employed, which is common and effective [1].
First, the experimental analysis was made for three concrete beams (40x40x160 mm^3) with a notch (4x7 mm^2) in the middle part. Support spacing was chosen as 120 mm. All beams were made of a concrete mix consisting: CEM I 42.5R (450 kg/m^3), water (177 kg/m^3), sand 0-2 (675 kg/m^3) and gravel 2-8 (675 kg/m^3). The bending test was carried out on Zwick/Roell Z10 universal testing machine. The elastic waves caused by cracking concrete were sensed using four piezoelectric transducers, arranged in a 2x2 grid. They were located on both sides (left and right) from the notch in the distance of 50 mm, at 10 mm and 30 mm in height (on the front side of the beam). Data acquisition was carried out using the AMSY-6 system (Vallen Systeme GmbH). The loading was performed with a constant displacement rate of 0.05 mm/min (quasi-static conditions). The AE signals were recorded during whole tests, up to the final damage of the beams.

In parallel with laboratory tests, the numerical model was created. The discrete element method (DEM) was used since it directly simulates the material meso-structure. Thus it is suitable for comprehensive studies of mechanisms of the initiation, growth, and formation of localized zones, cracks, and fractures at the mesoscale [2]. It easily represents discontinuities caused by fracturing or fragmentation. The open-source code YADE [3] was employed for calculations. Three samples were created, based on the real geometry (from the photo). Due to calculation time, the numerical study was limited to the 2D problems only (one layer of grain). The concrete was simulated as 4 phase material, consist aggregate, interfacial transition zone (ITZ) around them, air voids and cement matrix [3]. The cement matrix was filled specimen in 97% (thus microporosity was equal to 3% as in the experiment). The air voids were simulated as empty spaces. The aggregates were composed of spherical elements with cohesion, which can break in contrast to the last calculations, where they were simulated as non-breakable clumps. The shape and position of the aggregate were taken directly from photos of laboratory beams. The numerical parameters were calibrated on uniaxial compression and tension [3]. Each specimen contained more than 30'000 elements (with a coordination number of about 7). The elastic wave was recorded during the test in the same places as in the experiments.

The force-deflection (and CMOD) curves were compared, and good agreement was found between laboratory tests and numerical calculations. Also, the shape of the final crack (determined experimentally by the digital image correlation technique) was similar in both cases. The results obtained on all transducers were also compared directly with laboratory tests, with good agreement. The non-destructive AE method has shown to be a good tool for early-stage damage detection. Moreover, the DEM method shows a great ability to successfully model the elastic wave during the fracture process. In future work, the 3D calculations on real geometry are planned.

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Mesoscale discrete model for monotonic, cyclic and fatigue loading of concrete

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The task of predicting the structural performance of concrete, including its damage and failure, is very practical one and it has led to a number of innovative models and modeling approaches. The limitations of traditional fracture mechanics to properly capture quasi-brittle behavior of concrete is one of the driving forces behind the development of advanced modeling approaches. These models must balance the incorporation of material features that dictate the concrete behavior with the computational tractability, because in the end, models should not only serve to improve scientific understanding of the underlying phenomena, but most importantly to solve practical problems. The available advanced models range from modified *continua* in which the heterogeneity is modeled via spatially varying properties to *discrete* models in which the material representation is better tied to the physical microstructure and the micromechanical phenomena that produce quasi-brittle behavior.

The last about two decades has seen a gradual rise in discrete models that use discontinuous representations of the quasi-brittle material. The particle-based discrete models resolving the mesoscale features (individual large mineral grains) seem to provide the best balance between affordable computational complexity and the amount of captured structural redistribution effects associated with inelastic effect in heterogeneous materials such as concrete. The advantage of discrete models is the possibility to use vectorial-based constitutive law for individual interfaces instead of full tensorial description needed in standard continuum-based models. The triaxial stress redistribution effects with complicated phenomena such as anisotropic damage are automatically captured by the resolution of material mesoscale with the involved interactions between material bonds described by interface-like constitutive laws, see e.g. a recent advanced damage-plastic interface model presented in [1]. The marriage of the tractable vectorial description with structural effects is the key to success in matching diverse mechanisms in a wide range of loading scenarios.

The particle-based discrete model used in the present work reproduces the material integrity via mechanical components (links) each representing the connection between a pair of two adjacent mineral grains. A phenomenological interface model is used to lump the inter-aggregate interaction into a single interface constitutive law. This constitutive model must, apart from the variety of monotonic loading scenarios, respond reasonably also under cyclic loading.

This presentation serves as promotion of a recent work [2] focused on mesoscale modeling of concrete, in which we show that a single discrete model with a properly formulated constitutive law featuring a combination of damage with plasticity is capable of reproducing experimental data obtained on concrete under: (i) monotonic loading with both proportional and non-proportional loading, (ii) cyclic loading (postcritical cycling leading to low-cycle fatigue), and (iii) fatigue loading (precritical cycling leading to high-cycle fatigue). In this way, a common approach for a general monotonic, cyclic and fatigue loading is established. The model provides the history of energy dissipation, and the detailed energy breakdown allows for the analysis of the link between the dissipation generated by the cyclic plastic activity and the crack initiation via damage.

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Discrete modeling of concrete failure and size-effect

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Size-effect in concrete and other quasi-brittle materials defines the relation between the nominal strength and structural size when material fractures. The main cause of size-effect is the so-called energetic size-effect which results from the release of the stored energy in the structure into the fracture front. In quasi-brittle materials and in contrast to brittle materials, the size of the fracture process zone is non-negligible compared to the structural size. As a consequence, the resulting size-effect law is non-linear and deviates from the response predicted by linear elastic fracture mechanics. In order to simulate the size-effect, one needs to rely on numerical modeling to describe the formation, development and propagation of the fracture process zone. Although a number of models have been proposed over the years, it transpires that a correct description of the fracture and size-effect which accounts for boundary effects and varying structural geometry remains challenging. In this study, the Lattice Discrete Particle Model (LDPM) [1] is proposed to investigate the effects of structural dimension and geometry on the nominal strength and fracturing process in concrete. LDPM simulates concrete at the aggregate level and has shown superior capabilities in simulating complex cracking mechanisms thanks to the inherent discrete nature of the model. In order to evaluate concrete size-effect and provide a solid validation of LDPM, one of the most complete experimental data set available in the literature [2] was considered and includes three-point bending tests on notched and unnotched beams. The model parameters were first calibrated on a single size notched beam under three-point bending and on the mechanical response under unconfined compression. LDPM was then used to perform blind predictions on the load-crack mouth opening displacement curves of different beam sizes and notch lengths. Splitting test results on cylinders were also predicted. The results show a very good agreement with the experimental data. The quality of the predictions was quantitatively assessed. In addition, a discussion on the fracturing process and dissipated energy is provided. Last but not least, the Universal Size-Effect Law proposed by Bažant and coworkers [3] was used to estimate concrete fracture parameters based on experimental and numerical data. The proposed approach and results were first presented in a recent conference [4] and were later published elsewhere [5].

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Adaptive refinement for discrete models of coupled mechanics and transport in concrete

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Mesoscale mechanical models represent a reliable and robust approach to modeling of pre- and post-critical mechanical response of concrete structures. The composite material is represented by an assembly of rigid bodies interconnected by cohesive contacts. The kinematics of the model is derived from the rigid body motion, as proposed in [1]. These models are capable of capturing discrete jumps in the displacement field and therefore are suited for simulating of fracture. At the contact facets, a vectorial constitutive formulation is used, providing a simpler approach than the traditional tensorial formulation. Inherently, this formulation also yields the orientation of cracks.

In this work, an adaptive refinement algorithm for steady state discrete mesoscale models is presented, accounting for the coupled mechanics and mass transport in concrete. The coupling is based on two phenomena: (i) the Biot's theory and (ii) the influence of cracks on the material permeability. The model kinematics is derived from rigid body motion of the Voronoi polyhedra resulting from the tessellation of the model volume.

Initially, the model is represented by a coarse non-physical discretization and during the solution, its selected regions are refined to meso-scale discretization as they approach the nonlinear regime. At the solution beginning, only an elastic behavior is assumed and therefore it is not necessary to keep track of the loading history or state variables. The density of the particles (Voronoi generator points) is adaptively refined during the numerical solution. Whenever the state of any of the rigid particles starts to approach a selected threshold, the neighborhood of the particle is refined.

The refinement criteria and the size of the neighborhood are input parameters. Various failure/refinement criteria can be found in the literature, see e.g. [2] and [3]. As a suitable refinement criterion, we propose using e.g. 70% of the material tensile strength as used in [4]. Once a region has been refined to the fine (mesoscale) discretization, another refinement is prohibited as nonlinear behavior is expected to develop.

In [4], an adaptive refinement was proposed for mechanical models. In the presented work, we extend this concept for two-way coupled models of mechanics and mass transport in saturated heterogeneous solids such as concrete.

The adaptive geometry update provides a major decrease of the number of degrees of freedom. A comparison of solution performance is presented using various numerical models representing diverse modeling use-cases. Typically, a speedup of about 10-12x can be achieved depending on the specific modeling scenario. It is shown that the adaptive refinement algorithm can be employed for coupled discrete mesoscale models and provides a significant solution speedup.

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Homogenized mesoscale discrete model for coupled mechanics and mass transport

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Mesoscale discrete models of heterogeneous quasibrittle materials have been are under development for several decades [1]. They are often used for simulations of fracture processes, because the discrete nature of the model allows for direct representation of oriented discontinuity. The mesoscale character of the model brings detailed information about the creation of microcracks, transition from diffused to localized cracking process, and/or propagation of the macrocrack. For these reasons they are perfectly suited for coupling with the mass transport phenomenon. The original isotropic permeability tensor rapidly changes by several orders of magnitudes with the development of cracks and becomes highly anisotropic. The coupling scheme is typically adopted according to Refs. [5], where the primary geometrical network is used for mechanics and the dual network solves the mass transport.

The mechanical model is adopted from Ref. [2] and is slightly modified. The coupling with the mass transport in saturated medium is provided by four components: the Biot's theory where (i) the effective traction at the discrete contacts is composed of the traction in the solid and the fluid pressure contribution and (ii) the rate of the volumetric deformation is linked to the fluid pressure; (iii) the cracking which enhances the permeability coefficient of the associated conduit elements; (iv) the open cracks create storage space for the fluid.

There is, however, one disadvantage associated with the mesoscale character of the model – a large computational burden. To address this issue Rezekhani and Cusatis [6] developed an asymptotic expansion homogenization capable to separate the macroscopic trends and mesoscale fluctuations. The macroscopic model becomes homogeneous Cosserat continuum solved by the finite element method. Every integration point of the macroscale contains, instead of the constitutive routine, an embedded sub-scale model of periodic unit cell, so called RVE. The same approach is taken in Ref. [4] to homogenize discrete problem of mass transport (or diffusion or conduction as they have an identical mathematical structure).

The contribution extends previous separate homogenizations of the mechanics and mass transport to account for the coupling effects. It as a brief summarization of the recent article [3] of the authors.

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Spherical representative volume element for discrete mesoscale model of concrete

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Fracture in concrete occurs as a result of the interaction between aggregates and surrounding matrix. However, when modelling concrete structures, the common approach is to consider the structure as a whole and the material as homogeneous. Consequently, behavior of the structure at lower scales is not being explicitly included.

One way to capture intrinsically multiscale phenomena in models without adding insupportable computational costs is via homogenization, which allows to couple behavior between two (or even more) scales. In the case of concrete, the coupling is done between mesoscale, where fracturing occurs, and macroscale, where calculations are usually done.

The cornerstone to any homogenization scheme is a representative volume element (RVE) [1], which serves as a statistically representative sample of a material at mesoscale, attached to the integration point in the macroscopic framework and serving as a constitutive law. Loading of the macroscale structure is transferred onto the RVE via boundary conditions, which mimic the matter surrounding the RVE.

Among other options, periodic boundary conditions (PBCs) are used for the purpose most often [2], as they have been shown to not affect the RVE stiffness, contrary to other BCs [3]. PBCs presume a periodically repeating block of material, whose kinematics is restricted by the periodicity. When applied to a single RVE, it translates into constaints between nodes on opposing sides of a RVE.

Commonly, the shape of choice for a RVE is a square (2D) and a cube (3D), because they may periodically fill a space [3]. When dealing with materials experiencing strain localization and subsequent fracturing, applying PBCs to a cubical RVE is problematic. During softening, the constraint between opposing nodes introduces spurious material anisotropy and the RVE looses representability, crucial for homogenization.

To overcome the problematic aspect described above, mostly some form of a shift or a rotation have been introduced to align constraint with the desired direction of emerging crack [2]. A possible unconventional solution to the problem is offered by a shape change of the RVE [4].

By employing circular (2D) or spherical (3D) representative volume element, PBCs may still be applied, because periodic filling of a space is not in fact required in homogenization [3]. Instead, the application of PBCs assumes opposite normals to the RVE surface on opposing sides, which spherical RVE fulfills. Centrally symmetrical distribution of nodes at the surface of the RVE than allows straightforward rotation of the coordinate system. RVE of such a form is of itself immune to the shape dependency.

The present contribution aims to introduce primary results obtained with a circular RVE consisting of a lattice discrete particle model of concrete (LDPM). Firstly, the creation of a geometry and the implementation of classical PBCs is described, specifically considering discrete model. Subsequently, the performance of the circular RVE is compared with the common square RVE, with the emphasis placed on the size effect of the RVE and convergence.

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Numerical modelling of thermoset polymers

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Predicting the bonded anchors' response to various loading is very challenging since different material types are involved, i.e. concrete, thermoset polymer and steel. The paper presents the development of a material model utilized to characterize the behaviour of particulate thermoset polymers. The numerical model is based on the lattice discrete particle representation [1] to capture the particle distribution, size and material properties together with the ability to simulate thermosets on the scale of application.

The Lattice Discrete Particle Model (LDPM) simulates the material as a collection of rigid bodies (cells) interacting over the facets defined between them. These facets are assumed to be in the matrix phase between the adjacent cells and are interpreted as potential crack surfaces. The system of polyhedral cells is created based on the grain distribution curve. Note that there are different options utilized for the LDPM internal structure generation, see [1] or [2]. Each cell consists of the aggregate and surrounding matrix phase found between the particles. Contrary to the original LDPM formulation, no mix design is needed for particulate polymers, and only the distribution of filler sizes is assigned.

The following items characterise the constitutive law:

- The compressible generalised Leonov model is utilised to characterise the viscoelastic material behaviour of polymers.
- The volumetric-deviatoric is utilised to capture the Poisson ratio, which is typically above 0.25 for this type of material. Note that the Poisson ratio is restricted to a maximal value of 0.25 for standard LDPM formulation.
- The nonlinear behaviour captured by the proposed numerical model further includes fracturing, material compaction and frictional behaviour.

The numerical model is compared with the standard experimental tests.

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Discovery of damage tolerant quasi-disordered truss metamaterials inspired by natural cellular materials

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Natural cellular materials, such as marine mussels, honeycombs, woods, trabecular bones, plant parenchyma, sponges and protoreaster nodosus, have inspired the development of mechanical metamaterials with desired or extreme mechanical properties. These include various truss-like micro-lattices, i.e., truss mechanical metamaterials, at a scale ranging from nanometres to millimetres, manufactured using various additive manufacturing techniques. Truss metamaterials have provided unique opportunities to create lightweight structural components of high performance, such as lightweight sandwich structures [1,2]. In addition, truss metamaterials are highly tailorable and can be designed to meet various multifunctional requirements, such as simultaneous load bearing, active cooling, and noise reduction.

Up till now, the majority of the relevant research has focused on the truss mechanical metamaterials of highly ordered structures, i.e., the bulk metamaterial is formed by repeating a representative volume element (RVE) in the two-dimensional (2D) or the three-dimensional (3D) space. However, while nature-provided cellular materials resemble truss lattice structures of ordered, periodic arrangement, they are not perfectly periodic, and disorderliness has been observed in a wide range of natural cellular materials [3]. Natural cellular materials may benefit from the disorderliness within their internal microstructures to achieve damage tolerant behaviours. Inspired by this, we have created quasi-disordered truss metamaterials (QTMs) via introducing spatial coordinate perturbations or strut thickness variations to the perfect, periodic truss lattices. Numerical studies have suggested that the QTMs can exhibit either ductile, damage tolerant behaviours or sudden, catastrophic failure mode, depending on the distribution of the introduced disorderliness. A data-driven approach has been developed, combining deep-learning and global optimization algorithms, to tune the distribution of the disorderliness to achieve the damage tolerant QTM designs. A case study on the QTMs created from a periodic Face Centered Cubic (FCC) lattice has demonstrated that the optimized QTMs can achieve up to 100% increase in ductility at the expense of less than 5% stiffness and 8%–15% tensile strength. Our results suggest a novel design pathway for architected materials to improve damage tolerance.

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An efficient 3D crack propagation model using the total Lagrangian smoothed particle hydrodynamics with a frame of reference update

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The total Lagrangian version of the smoothed particle hydrodynamics (TLSPH) offers many advantages over the classical updated Lagrangian version. The TLSPH provides better stability, and computational-time cost, which the tensile instability is vanished using TLSPH, and the neighbour search is only once at the first time step, making the computational time shorter. However, in the application of fatigue crack propagation with the presence of geometry change, a pure total Lagrangian formulation is not capable of handling the problem. The interaction pairs of the particle, especially near the crack tip, must be updated. On the other hand, if the updated Lagrangian formulation is used, this problem can be handled well with the consequence of higher computational time costs. Therefore, an efficient 3D crack growth modelling using the total Lagrangian smoothed particle hydrodynamics with an update of the frame of reference is proposed.

The development of the SPH method for fatigue crack propagation still becomes an interesting research area. One of the latest publications is the pseudo-spring based SPH for fatigue crack simulation [1]. In our previous research, the TLSPH is proposed for 2D fatigue crack growth simulation [2]. To handle the geometry change in the crack growth problems, the interaction pairs at the crack tip are deactivated when the crack propagates, and the stress distribution is returned to zero. The direct deactivation of the interaction pairs when the crack propagates yields the kernel gradient of its neighbour remaining the same with the initial value without a new correction when the geometry change. This problem will affect the completeness of the SPH approximation at the crack tip. Therefore, a further improvement for TLSPH is required in the application of crack propagation simulation. In this research, the previous crack growth model for TLSPH is improved using an update of the frame of reference every time the crack propagates. The interaction pairs are deactivated when the crack propagate, which is similar to the previous research. In order to maintain consistency and completeness, kernel gradient correction using the update of the frame of reference is proposed. On the newly geometry with a crack extension, the particle's coordinate is transformed to the undeformed configuration. Then, the kernel gradient is recorrected on the new updated frame of reference. Then, the simulation is continued to obtain a new stress distribution.

The proposed crack model in this research is applied for 3D fatigue crack growth simulation. The crack is modeled using a surface that propagates through the particle interaction. An efficient procedure to calculate 3D J-integral for SPH is presented. Then, the stress intensity factor can be calculated using the relation of energy release rate and J-integral in LEFM problem. The maximum normal stress or maximum shear stress criteria can be used to determine the orientation of the new crack plane, depending on the material properties, load configuration, and the dominating crack mode during the propagation process. Finally, the results are compared with available data in the literature.

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Transition State Theory based Thermally Activated Breakdown in Fiber Bundles: Exact Solutions and Asymptotics for the Lifetime Distribution, Average and Variance

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Fiber bundles serve are the easiest model used to describe the statistical aspects of failure and fracture. For the special case of thermally activated failure in creep a model based on stationary Gaussian thermal noise in the form of additional force fluctuations has been introduced by Guarino for the equal load-sharing force fiber bundle [1]. Roux provided the exact solution for the average lifetime and the asymptotics of average and variance in the limit of many fibers and low temperature for a homogeneous fiber bundle [2]. However the assumption of a Boltzmann like distribution has been analytically difficult to handle and bears little empirical basis.

A new fiber bundle model based on transition state theory is established [3]. The failure rate of individual fibers is given by an Arrhenius relationship with an energy barrier linearly lowered by the applied force. Thermally activated fiber failure is assumed follow the usual Poisson process. for an arbitrary number of fibers the lifetime distribution, average and variance can be solved exactly. The asymptotic limit for many fibers reveals a constant average lifetime and the variance decreasing inversely proportional to the number of fibers. The exact and asymptotic expression agree perfectly with simulations. The low temperature limit by Roux shows the same with respect to the number of fibers, but a different relationship with regards to applied force and temperature is found [2]. For heterogeneous fiber bundles, the lifetime distribution is shown to be a high dimensional integral over a phase type distribution with no elegant closed form expression. For fiber strengths distributed according to uniform an exponential distributions, simulations show the lifetime average and variance to behave identically in the asymptotic limit of many fibers as bundles of the homogeneous fiber bundle. The lifetime does have a strong dependence on the details of the fiber threshold distribution. Preliminary results with regards to the asymptotic avalanche distribution will be presented which suggest a power law scaling of exponent 1.5 as has been derived by Hemmer for the quasistatic case [4].

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Minisymposium EFE:

Enriched finite element formulations for fracture

Organized by J. Alfaiate and L. J. Sluys

3-D Modeling of Multi-Stage Hydraulic Fracturing from a Borehole within a GFEM Framework

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Hydraulic Fracturing is the process in which a fracture propagates through the injection of pressurized fluid in its cavity. This process is widely used in the oil and gas industry to increase reservoir permeability which leads to high rates of both injection and production. In order to reduce operational costs, hydraulic fractures are usually created in stages where multiple fractures are propagated at the same time [1]. Interactions among fractures and their realignment with the preferential propagation direction often lead to complex fracture geometries. The fracture shape, and consequently pressure drop, varies significantly between fractures which can impact their productivity. Miller et al. [2] studied more than 100 horizontal shale wells in multiple basins and concluded that an average of 29.6% of the hydraulic fracture clusters do not produce. Computational methods able to predict the near-wellbore tortuosity and pressure drop can play a key role in improving the performance of multistage fracturing.

This presentation reports on recent advances of an adaptive Generalized Finite Element Method (GFEM) for the simulation of multiple 3-D non-planar hydraulic fracture propagation near a wellbore [3]. This method is particularly appealing for the discretization of the fractures since it does not require the finite element mesh to fit fracture faces. Additionally, analytical asymptotic solutions are used to enrich the fracture fronts, which increases the accuracy of the approximation. The governing equation of the rock is discretized in space with a quadratic GFEM and the equation for the flow in the fractures is discretized in space with a quadratic FEM. The injected fluid partitioning among fractures is automatically computed by modeling the wellbore, where the flow is assumed to be governed by the Hagen–Poiseuille relation. The pressure losses between wellbore and hydraulic fractures are modeled with the sharp-edged orifice equation and with the use of 1-D connecting elements. A linear FEM is adopted for the spatial discretization of the equation governing the flow in the wellbore and the connection between wellbore and hydraulic fracture. A propagation criterion based on a regularization of Irwin's criterion is adopted and a methodology to automatically estimate the time step that leads to the propagation of fractures based on linear interpolation/extrapolation is presented.

Several wellbore and fracture configurations are investigated to demonstrate the non-intuitive propagation behavior in these near-wellbore conditions and the robustness of the proposed GFEM methodology. They show that even a fairly small misalignment between the wellbore and the minimum in-situ stress leads to fracture geometries that are vastly different from those predicted by simulations that assume fracture planarity – a simplification often adopted in the simulation of hydraulic fractures propagation.

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Modeling combined necking cracking phenomena using different modeling techniques

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Ductile fracture of metals is characterized by the formation of highly localized zones of intense straining which ultimately leads to the onset of fracture and failure. Presence of two interacting localization phenomena, necking and cracking in ductile fracture is observed in different experiments performed on thin metal sheets under different loading conditions [2]. This contribution aims to model the interaction of necking and cracking phenomena using different modeling techniques. While incorporating necking and cracking phenomena into a failure model, attention will be given to the local deformation and stress state in a neck or ahead of a crack tip, and also the global behavior such as boundary conditions and force displacement behavior. The first modeling technique that is incorporated to simulate necking cracking interaction uses a continuum approach to model necking followed by XFEM integrated into a geometrically nonlinear discontinuous solid-like shell element [1] to simulate fracture and ultimately failure. Although this technique is helpful to model details of necking deformation (both in-plane and out-of-plane), the model suffers from mesh dependent behavior while modeling necking phenomena. The second modeling technique in this contribution uses a discontinuous approach for both localization phenomena. The transition of a neck to a crack is governed by a fracture initiation model and different segments of the traction separation law. This technique is advantageous for reproducing the global force-displacement behavior and reducing mesh dependence. The traction separation law that governs the failure process zone after initiation of XFEM plays a significant role in the failure modeling. The effect of different parameters and shapes of traction separation laws in simulation of interaction of necking and cracking phenomena using both modelling techniques is thoroughly investigated in this contribution.

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An eXtended IGABEM formulation for the direct determination of SIFs in three-dimensional cracked bodies

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The Boundary Element Method (BEM) has been successfully applied in various fracture mechanics problems, since it can accurately capture mechanical fields in discontinuous problems. Moreover, once the method requires a boundary-only mesh, the remeshing process is simplified for crack growth analyses. In addition, its coupling with the isogeometric analysis concept becomes straightforward, in which the same parametric curves used in Computer-Aided Design (CAD) software also represent the interpolation of mechanical fields. As a result, the Isogeometric BEM (IGABEM) arises as a powerful tool to determine the mechanical response of solids and structures, for both elastostatics [1-2] and fracture mechanics [3-4].

On the other hand, it has been a challenge to simulate three-dimensional fracture mechanics applications when the crack intersects the external boundary using IGABEM. In such a scenario, it is necessary to carefully create the geometry by placing the NURBS patches so that they will not be crossed by the crack, to generate a discontinuous mesh. However, this approach can be unfeasible, depending on the crack's position. To overcome this issue, this presentation will describe an eXtended IGABEM (XIGABEM) formulation in which the strong discontinuous displacement field is naturally introduced by a Heaviside enrichment. Then, additional unknowns represent the crack opening at the crossed patch, which requires a technique to generate additional equations.

Besides, standard BEM and IGABEM formulations are not capable of describing accurately the displacements near the crack tip. Neither the standard polynomials nor the NURBS used in IGABEM offer an efficient approximation of the $1/\sqrt{r}$ behaviour in this location. In fact, at the crack tip, the solution given by the method contains non-physical displacement discontinuity at the crack front. This problem is herein circumvented by using the crack tip enrichment based on the Williams solution. Once the additional unknowns are the Stress Intensity Factors (SIFs), this technique also allows us to directly determine them from terms in the solution vector, which becomes another advantage of the XIGABEM. It is worth mentioning that the direct evaluation of SIFs is significantly more efficient than J-integral in terms of computational effort and more accurate than other procedures, such as Displacement Extrapolation Technique.

In this context, this presentation will discuss the methodology and results associated to a three-dimensional XIGABEM formulation for a pure mode I fracture mechanics application. Therefore, it will be possible to attest the robustness and accuracy of the developed techniques.

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A Discontinuity-Enriched Finite Element Method for Crack Growth in Brittle Materials

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The standard finite element method (FEM) can be used to model brittle fracture, but cracks have to be aligned with edges of finite elements. As an alternative, the eXtended/Generalized Finite Element Method (XFEM/GFEM) elegantly decouples the crack geometry from the discretization [1]. However, some important properties of standard FEM are lost, e.g., the condition number of the stiffness matrix can be arbitrarily high when cracks are very close to standard FEM nodes, and standard degrees of freedom (DOFs) loose their physical meaning. The computer implementation is also far from trivial, since non-standard procedures are required for prescribing nonzero essential boundary conditions (BCs) when enrichments are nonzero along Dirichlet boundaries (e.g., shifting or penalty formulations). Finally, the formulation is very intricate when dealing with complex discontinuity cases such as branching and merging.

As an alternative to XFEM/GFEM, the Discontinuity-Enriched Finite Element Method (DE-FEM) [2, 3] can solve problems with both material interfaces and cracks and with a unified formulation. DE-FEM places enriched DOFs to nodes created directly along discontinuities, thereby solving many issues of XFEM/GFEM. Because enrichment functions in DE-FEM vanish at standard mesh nodes, standard DOFs retain their physical meaning and there are no issues in blending elements. The method is also stable with regards to the condition number, and nonzero essential BCs can be enforced strongly. Finally, DE-FEM's computer implementation in displacement-based FEM codes is straightforward. DE-FEM thus keeps the most salient feature of XFEM/GFEM—decoupling between mesh and cracks—while retaining some desirable properties of standard FEM.

DE-FEM has only been studied so far for stationary cracks under stationary loading cases. In this presentation, we demonstrate DE-FEM for both quasi-static and dynamic brittle fracture propagation, including branching and merging. For dynamic fractures, implicit time integration methods are used and their parameters are tuned to mitigate numerical instabilities. Dynamic stress intensity factors are obtained by a path-independent dynamic interaction integral [4] and propagation directions are determined according to maximum circumferential stress criterion. The methodology is demonstrated on a set of complex crack growth problems.

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The Shifted Fracture Method

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We propose the Shifted Fracture Method (SFM), a new framework for computational fracture mechanics, which is based on the idea of an approximate fracture geometry representation combined with approximate interface conditions.

Our approach evolves from the shifted boundary method [1] and the interface method [2], and introduces the concept of an approximate fracture surface composed of the full edges/faces of an underlying grid that are geometrically close to the true fracture geometry. The original interface conditions are modified on the surrogate fracture, by way of Taylor expansions, to achieve a prescribed level of accuracy.

The SFM does not require cut cell computations or complex data structures, since the behavior of the true fracture is mimicked with specific integrals on the approximate fracture. Furthermore, the energetics of the true fracture are represented within the prescribed level of accuracy and independently of the grid topology.

The computational framework will be presented in its generality and then applied in the specific context of cohesive zone models, with an extensive set of numerical experiments.

We demonstrate in particular how the SFM correctly captures the energy released as the fracture propagates, independently of the grid geometry.

We also show how the SFM can be combined with phase-field approaches to simulate crack branching and merging.

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Inelastic analysis of frames using thin beam-column elements with multiple embedded plastic hinges

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The development of a variational formulation of the mechanical behavior of thin beam-columns with multiple embedded plastic hinges is developed. The boundary value problem, which is valid throughout the domain of the structural member, is obtained from the proposed formulation that provides the necessary tools to deal mathematically with the singularities. The plastic hinges are modelled as strong embedded discontinuities, which are adapted to represent the strain localization. These embedded discontinuities represent the material failure process as hinges for beams and cracking or crushing for bars, in which a displacement jump, and the stain concentration are lumped into a zero-thickness localization zone. The non-linear behavior of the materials is described by a multilinear plasticity model.

Closed form solutions for bars [1] and thin beams [2] with strong embedded discontinuities are obtained by solving the proposed formulation. From these solutions, bar and beam finite elements with embedded discontinuities are developed, which model the occurrence of damage in frame elements. Based on conventional procedures of structural analysis and the developed closed form solutions, a symmetric stiffness matrix of a thin beam-column element with multiple strong embedded discontinuities with arbitrary locations is developed. This matrix is naturally condensed, its coefficients are not in terms of integrals and any type of loads can be modelled, which reduce the computational cost and avoid possible numerical instabilities [3].

Representative examples of beams and frames validate the capability of the formulated thin beam-column element for modelling damage. In these examples, the load-displacement curves agreed with those reported in the literature. The induced work on a structure is adequately release as energy in the development of hinges in the thin beam-column element. The computed solutions with the developed element are mesh independent because the same results were computed with different meshes. This developed element adequately models the snap-back behavior in frames. Finally, it is important to mention that this element is able to model multiple hinges per element; therefore, only one finite element is required per structural member.

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Multiscale Extended Finite Element Method for Simulation of Fractured Geological Formation with Propagating Fractures

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When the equilibrium state of geological fractured formations is violated, fractures can propagate and slide. This change of in-situ stress state can often be activated by an injection or production process. Due to the compressive nature of the stress state in underground formations, mode II mechanical failure, or shearing, is the dominant fracture propagation mechanism while opening fractures can be barely seen. In addition, massive fractures often cross each other in the fractured formations. To avoid the use of excessively high-resolution meshes, while resolving the explicit fractures, the extended finite element method (XFEM) is used [1]. The XFEM introduces jump functions to enrich the FEM continuous space with discontinuities introduced by the fractures. The linear momentum balance equation is then supplemented by the Mohr-Coulomb friction law, which defines the maximum friction that each fractured element can tolerate. Further constraints are applied to ensure that no penetration of elements takes place as a result of significant deformations [2].

For the simulation of highly fractured geological formations, applying XFEM directly is computationally challenging. The large number of extra degrees of freedom (DOFs) due to the highly fractured formations will cause high computational burden. To resolve this challenge, we propose this multiscale extended finite element method (MS-XFEM) to simulate fracture propagation under compressive loading in geological formations. Local XFEM-based basis functions are constructed algebraically to capture the compression and the sliding of fine-scale fractures [3]. In each time step when the fractures propagate, the basis functions are updated adaptively in certain regions where fractures geometries are changed. Using these basis functions, a very efficient FEM-based coarse-scale system is developed since it has no extra DOFs. Once the coarse-scale solution is obtained, it is prolonged to the fine-scale original resolution using the basis functions. This approximate fine-scale solution is then used to estimate the group of growing fracture tips and their growing angles. This allows for exploiting the locality of the propagation process fully while solving a global system. To control the error, an iterative procedure is also developed. MS-XFEM casts a promising method for field-scale applications.

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Virtual element method for mixed-mode cohesive fracture simulations

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The Virtual Element Method (VEM) has attracted a lot of interest from the scientific community and numerous results have been achieved in different research fields, comprising linear elasticity problems, inelastic problems, fluid-flow problems and contact problems [1]. In particular, VEMs can be conveniently applied within the context of computational fracture mechanics.

In this field, the numerical approaches proposed in literature are mainly based on the finite element method (FEM) or on modified forms of this latter such as the extended FEM and the augmented FEM.

The VEM formulation is characterized by the possibility to define polygonal meshes with elements characterized by any number of edges and by the flexibility in mesh generation that allow to introduce a crack just redefining the element in two different elements joined by a crack modelled with an interface element. The features of the VEM appear particularly suitable for the development of a procedure able to follow the crack propagation in a solid, requiring a minimal remeshing [2].

The present work proposes an algorithm of nucleation and growth for fracture evolution in 2D cohesive media. The procedure is based on virtual element method specifically referred to a 4-side 12-node virtual element with piece-wise linear approximation of the displacement field on the edges. The large number of nodes and, consequently of degrees of freedom, is exploited to enrich the strain field evaluation. It is derived by means of the minimization of the complementary energy within the single element. This procedure allows to avoid the stabilization of the element stiffness matrix.

The fracture is introduced in the solid domain by splitting the virtual element, called parent element, into two slave elements, joined by a cohesive interface. The presence of the two nodes inside any edge of the parent element has been proposed for avoiding the generation of new nodes during the crack evolution. The obtained slave elements are characterized by a different number of nodes depending whether the straight crack within the parent element crosses two opposite or adjacent sides. At the interface, a cohesive law governed by a damage variable in mode I, in mode II and in mixed mode, and that takes into account for the unilateral effect due to the reclosure of the crack in compression, is adopted [3].

Moreover, the fracture direction is defined as the orthogonal to the maximum tensile principal nonlocal stress evaluated around the crack tip for the fracture growth, and in the element center for the nucleation. The maximum tensile principal nonlocal stress is computed averaging on the mesh, by means of a weight function, the stress field evaluated via complementary energy within each element.

Numerical simulations of experimental tests are developed in order to assess the ability of the proposed procedure to satisfactorily reproduce the crack nucleation and growth. The simplicity of the procedure with respect to other more complicated approaches is remarked highlighting the reduced computational effort and storage memory required.

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A new approach to model softening in quasi-brittle materials

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In quasi-brittle materials, such as reinforced concrete, masonry and glass, localisation of initially diffuse cracking is difficult to model. The use of conventional iterative methods such as the Newton-Raphson and arc-length methods, can lead to convergence difficulties, often hard to overcome. Other non-iterative techniques, such as the Sequentially Linear Approach, although robust, do not correctly approximate the governing material law. In the present work, a new method is introduced, designated the Total Iterative Approach, in which the internal damage variables are updated iteratively. This approach has proven to be a powerful tool for the analysis of softening behaviour: it is both robust and correctly approximates the material law. Some examples are presented to illustrate the performance of the model.

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Minisymposium FDCL:

Fracture and damage of composites and laminates

Organized by P. P. Camanho, S. Hallett and J. Remmers

Capturing the Off-axis Response of Thin-ply Laminates

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The ability to simulate the response and obtain accurate strength predictions for multidirectional laminated composite components is of prominent interest in the aeronautical field, especially concerning notched components, which often appear in aeronautical structures (e.g., bolted, riveted sheets). In this work, focus is attributed to a novel composite system, thin-ply laminates (i.e., plies of thicknesses under 0.1 mm) that have been shown in the literature to present different fracture patterns compared to *"standard"* ones (i.e., plies of thicknesses over 0.1 mm). In the former case, final failure tends to happen in the form of a single fracture plane. This motivates the use of the phase field method (PF), nominally used for brittle fracture, following an equivalent single layer (ESL) representation for the composite laminated plate.

The feasibility and application of this method is evaluated on the basis of off-axis (i.e., referring to loading on a direction that does not coincide with one of the principal axes of orthotropy of the plate) open-hole tension of a multidirectional laminate based on the experimental results of [1]. Results obtained using the anisotropic PF model of [2], which uses a 2nd order structural tensor to account for anisotropic fracture energy, reformulated as in [3] to include specific considerations of the toughness of a composite laminate, are initially presented. A successful prediction of the experimental results both with regards to fracture plane (Fig. 1) and strength, with a maximum observed error in predicted strength of 4.8%, is achieved.

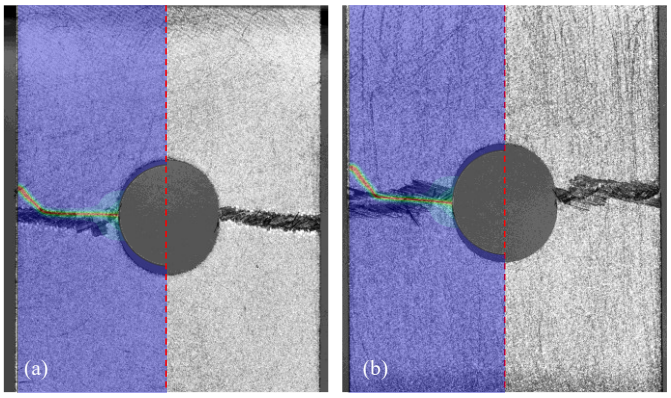

Fig.1 – Comparison of experimental and numerical crack paths for (a) 30º off-axis loading and (b) 60º off-axis loading.

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A Directed Continuum Damage Mechanics Approach to Model Static Indentation Induced Damage in Composites

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The demand for lightweight and high-strength materials in aerospace, automotive and marine industries has necessitated the use of fibre-reinforced polymeric composites in place of metal alloys. Existing structural design guidelines, therefore, need to be suitably modified considering the specificities in the mechanical behaviour of this new material system. Due to their inherent brittle nature, composite structures tend to fail catastrophically. This aspect is of particular concern to the transportation sector, where ensuring passenger safety is of utmost importance. Among others, low-velocity impact (LVI) is one of the common incidents causing localised damage in composites. Since LVI typically causes damage to the interior of the laminate and the exterior appears intact to visual inspection, it is also known as Barely Visible Impact Damage (BVID). Advanced structural health monitoring techniques are commonly required to identify the extent of this type of damage experimentally, which increases inspection cost and time. Computational realization of LVI events incorporating accurate damage models provides an alternate route to understand better this type of damage in an inexpensive way.

In a Finite Element (FE) framework, LVI-induced damage is commonly modelled at the ply level using continuum damage mechanics (CDM) framework, while interface damage is represented by cohesive zone models (CZM). However, the classical CDM method works by gradually degrading the material stiffness by smearing the damage across the entire element volume, resulting in the loss of information about the discrete nature of ply matrix cracks as well as the crack and delamination interaction during damage growth. Another issue with classical CDM is that the crack growth direction is influenced by the mesh lines of the finite element model [1]. To address the second issue, typically local fibre direction-oriented mesh is used for each individual ply of the laminate [2] which adds to the meshing effort significantly. Additionally, oriented mesh results in mesh mismatch at ply interfaces, requiring enforcement of tie constraints to hold the assembly together, which substantially increases computational time.

Since, quasi-static indentation results in a very similar damage pattern as observed under dynamic conditions in LVI [3], the present work numerically simulates damage onset and growth under quasi-static indentation in a multidirectional laminate [2] using a novel directed CDM (D-CDM) approach [1]. The D-CDM augments the traditional CDM by incorporating an accurate kinematic representation of the sharp crack topology of the ply matrix cracks at the constitutive level. Further, a crack tracking algorithm is applied that eliminates the mesh orientation bias of ply crack growth, which greatly reduces the meshing effort. Also, the analysis time is reduced due to the elimination of tie constraints. This technique is implemented as a 3D user-defined material in Abaqus/Explicit.

The numerical results using this new method are compared with experimentally obtained damage patterns reported in the literature as well as associated load-displacement curves, showing an excellent agreement.

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Dissipation at multiple length scales for improved delamination resistance

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Laminated composites can fail by delamination, that is the fast and possibly unstable propagation of cracks between the plies. Improving the delamination resistance of composite structures involves increasing the load levels associated to crack initiation and propagation, but also, and more importantly, making the crack propagation more progressive and stable to delay final failure of the structure.

The stability of crack propagation depends on the ratio between the energy stored in the structure and the energy dissipated by crack propagation. The first is a function of the material, geometry (including crack location) and loading conditions of the structure, while the second depends on the properties of the delaminating interface. As such, the first and main lever to ensure a progressive and stable crack propagation is the design at the structural scale, and in particular ensuring that the crack propagates towards zone of the structure where it can release little energy.

From the point of view of interface properties, two key parameters play a role in the delamination response, namely the maximum stress transferred by the interface, and the energy per unit surface required for complete interface failure, also known as the critical strain energy release rate. These two parameters contribute to define the characteristic process zone length, which increases linearly with increasing critical strain energy release rate, but decreases quadratically with increasing maximum stress [1]. If the process zone length is comparable to the characteristic problem dimensions, a gradual and stable crack propagation can be achieved.

The role of the maximum stress and critical strain energy release rate can be easily investigated through numerical simulations using Cohesive Zone Models (CZM), which describe the progressive failure of an interface via a traction/separation law involving both parameters. Typical values for delamination interfaces lead to process zone lengths of the order of a few millimeters [2], which is insufficient to provide gradual and stable crack propagation. For this reason, additional dissipation mechanisms, having small maximum stress and large critical strain energy release rate, should be designed to work in parallel with the initial energy dissipation mechanisms to provide crack stabilisation features. A typical example of such mechanisms consists in the creation of bridging ligaments across the cracked surfaces [3, 4].

In this work, the combined effect of dissipation mechanisms at different length scales on the response of composite structures with propagating cracks is simulated using CZM and a dissipation-driven algorithm [5] to ensure the correct representation of snap-back instabilities. Such simulation enable one to define the target CZM parameters for a desired structural response [6].

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Failure analysis and optimal design of thick-walled composite pipes under combined loading

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The main advantages of composite materials are their high stiffness, good strength-to-weight ratio, and excellent corrosion resistance. However, the disadvantages of lower performance data, regulatory requirements, complex design procedures limit the industrial implementation of composites.

In the current study we present a comprehensive failure analysis of thick-walled multi-layered filament wound pipes subjected to combined loading that includes bending.

The finite element model is developed to carry out the stress and failure analysis, and the model is validated by the comparison with the three-dimensional elasticity solution, and the results obtained using the laminated plate theory for different modes of the loading (internal and external pressure, axial and shear loading, torsion and bending) [1–5] .

It is worth noting that the analysis shows the applicability of the laminated plate theory approach for composite pipes under bending with 0^0 and 90^0 degrees winding angles only (with some additional limitations).

It could be concluded that the developed finite element model and three dimensional elasticity solution (taking the extensional shear couplings into account) shall be used for failure analysis and optimal design of multi-layered composite pipes under pure bending and consequently under combined loading.

The detailed parametric analysis (including effects of fibres orientation, stacking sequence, magnitude of loading and layer thickness on the structural performance of the pipe) is given, and it is followed by the failure analysis and optimal design recommendations based on the modified Tsai-Hill failure coefficients.

In addition, to find the suitable fibre angles for the multi-layered pipes under loading the safety zones were introduced. Safety zones show the allowable angles for the particular lay-up and magnitude and direction of the loading, providing a wider range of options, making the design process of the filament wound pipe faster and more reliable [6].

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Structural cohesive element for the modelling of delamination between thin shells without cohesive zone limit

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Delamination is a critical mode of failure that occurs between layers in a composite laminate. The cohesive element is a widely-used interface element based on the cohesive zone model for modeling delamination. However, cohesive elements suffer from a well-known limit on the mesh density – the element size must be much smaller than the cohesive zone size.

The earlier work in 2D [1] shows that when plies are modelled with C1 structural elements (i.e., Euler-Bernoulli beams) and the cohesive element is formulated to be conformal to the ply elements, delamination modelling can be done with meshes where element sizes are larger than the cohesive zone length. This allows the new structural element models to achieve significant computational speed-up over traditional, solid-based models. Based on this earlier work, a follow-up work, which used TUBA plate elements, successfully reproduced the same result on 3D delamination in Mode I [2]. However, the TUBA elements employ curvature degrees of freedom, which makes the imposition of general boundary conditions troublesome.

In the current work, a new C1 triangular Kirchhoff-Love shell element is chosen to model the ply. No curvature degree of freedom is needed as opposed to the case in [2]. The triangular shape is chosen for its flexibility of modelling arbitrary (sub-)domain geometries. The interfaces are modelled by conforming cohesive elements. The cohesive element will share the degrees of freedom and interpolation scheme of the neighboring ply elements and account for the ply thickness projection when calculating the separation vector.

The proposed method is verified and validated on the classical benchmark problems of Mode I, Mode II and mixed-mode delamination [3]. All the results show that the size of elements can be at least 2 times larger than the cohesive zone length without suffering from the huge strength overprediction as in the case of solid-element models. This would then allow the accurate modelling of delamination without worrying about the cohesive zone limit on mesh density. Therefore, a lot of computing time can be saved by the proposed method.

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A mesoscopic model to predict ply-failure mechanisms in fibre-reinforced composites

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Mesoscopic constitutive models employed to predict the mechanical response of fibre-reinforced composites at the level of the unidirectional ply are typically formulated under the small strain assumption. However, this assumption may become inadequate for situations where large deformations are observed in the material when it is loaded up to failure. It may be the case of load cases leading to a matrix governed response, especially in the case of fibre-reinforced thermoplastics, which have the potential to become important structural materials in aeronautical applications due to their recyclability. The visco-elastic–visco-plastic response of fibre-reinforced polymers has been addressed by the authors in [1].

However, it has been recently demonstrated in [2] that finite strains must also be appropriately accounted for in damage models to accurately predict the progressive failure behaviour of composites. Therefore, an approach based on the finite strain version of the smeared crack model introduced in [3] is discussed. The onset of transverse matrix cracking is evaluated by an invariant-based criterion and its evolution is described through an homogenisation-based kinematic description of the cohesive crack. An extrinsic mixed mode cohesive law is employed to deal with non-monotonic load-unload-reload conditions. The local cohesive equilibrium problem is formulated in the reference configuration, enabling a natural inclusion of the crack-plane re-orientation. The smeared crack model is combined with a continuum damage model formulated in terms of the Green-Lagrange strain tensor, to include longitudinal failure mechanisms. The implementation of this approach for finite element solution with Abaqus/Explicit is addressed. Some numerical examples are also presented to illustrate the applicability of this model in the prediction of experimentally observed phenomena.

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Microscale modeling of time-dependent failure in unidirectional composites under off-axis loading

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Testing unidirectional (UD) composite material under different off-axis angles allows for covering a range of different stress states with a single setup. When strain-rates and stress levels are also varied, complex failure behavior is exposed, particularly for thermoplastic composites that display a markedly time-dependent response. To investigate the characteristics of the failure behavior, this contribution presents a micromechanical framework for modeling off-axis failure of UD composites.

The micromodel is a representative volume element (RVE) defined as a thin slice oriented perpendicularly to the fibers. Periodic boundary conditions are set on the RVE, allowing for periodicity in microcracking as well [1]. The thermoplastic matrix is represented with the Eindhoven Glassy Polymer (EGP) material model [2], whereas a transversely isotropic constitutive model is used for carbon fibers [3]. It is assumed that the material undergoes finite deformations locally and in a homogenized sense, therefore the microstructure changes orientation during the loading process. A constant strain-rate with globally uniaxial stress is imposed on the material under an evolving off-axis angle by means of a dedicated arclength model [4].

To model failure of the composite material, interelement cohesive surfaces are inserted on the fly. A cohesive zone initiation criterion based on the local rate of deformation in the polymer matrix is proposed [5]. The model performance is compared with experiments on a thermoplastic UD carbon/PEEK composite system tested at different off-axis angles and strain-rates.

Next, the framework is applied to simulation of creep rupture. Although creep deformation due to the viscous nature of the polymer matrix can be represented with the EGP model, predicting creep rupture requires two additions to the framework. Firstly, the creep rupture process is triggered by inserting cohesive segments with a criterion based on the critical free energy of the polymer matrix. Secondly, viscous degradation of the cohesive surfaces is included in the formulation. The rupture time is defined as the moment when the homogenized creep strain-rate reaches a minimum value. The model results are again compared with experiments, performed at different off-axis angles, stress levels and temperatures. Finally, the effect of the change in RVE orientation due to finite deformations on the creep response is illustrated.

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A micromechanical model to study the rate-dependent failure mechanisms of carbon fiber reinforced polyvinylidene fluoride

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Carbon fiber reinforced polyvinylidene fluoride (PVDF) is a composite material that combines the high strength and stiffness of carbon fibers with the high temperature tolerance and excellent chemical resistance of PVDF. Due to these beneficial material properties, carbon fiber reinforced PVDF is used for energy transport in the offshore industry. Although the material is used in a variety of engineering applications, its failure behaviour is not very well understood.

To investigate the material response to different loading conditions, uniaxial tensile and compression tests were performed at different constant loading rates at different ambient temperatures. Also the orientation of the carbon fibers with respect to the loading direction was varied. Results from transverse loading experiments, i.e. when the fibers are oriented perpendicular to the loading direction, revealed that the composite exhibits brittle failure with a small strain at failure. Furthermore, the transverse tensile strength of the composite is much lower than the yield stress of bulk PVDF [1]. Analysis of the fracture surface of the tested specimens revealed bad adhesion between the carbon fiber and the PVDF matrix. Especially in loading cases where the matrix response is dominant, this results in poor performance of the composite.

To better understand the failure behaviour of carbon fiber reinforced PVDF at the fiber scale, a micromechanical model of the composite is used in finite element simulations. A 3D representative volume element (RVE) with a number of fibers embedded in a matrix is defined. The geometric properties of the microstructure, e.g., fiber radius and fiber volume fraction, are derived from microscopic scans of the composite. The fibers are modelled using a transversely isotropic material model. For an accurate description of the matrix, the intrinsic behaviour of PVDF is modelled using an elasto-viscoplastic constitutive model that is able to describe the rate-dependent behaviour of PVDF at different temperatures and under different loading conditions [2]. The bad adhesion between fibers and matrix is incorporated in terms of cohesive zone elements at the fiber-matrix interfaces. An appropriate traction-separation law is used to describe the constitutive response of the cohesive elements.

Periodic boundary conditions were applied in combination with a macroscopic uniaxial strain, as introduced in [3]. This enables the simulation of off-axis uniaxial loads on a unidirectional composite, using only a thin slice of the 3D RVE. Both tensile and compression loads were applied at different constant strain rates and for different temperatures, similar to the experiments. Finally, volume averaging theory is used to calculate the macroscopic stress, which is compared to the experimental stress-strain response.

The simulation results show that the model can adequately describe the temperature- and rate-dependent non-linear response of carbon fiber reinforced PVDF. Furthermore, the addition of cohesive zone elements enables the description of the brittle failure response of the composite at different loading conditions.

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Progressive damage analysis of natural fiber composite laminates: A computational micromechanical perspective

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Natural fibre composites regarding their inherent environmental and performance advantages have become an alternative to environmentally harmful synthetic materials. These kinds of materials can be helpful in controlling pollution problems. Besides, having advantages like recycling benefits, potential cost saving, good dimensional stability and reduced tooling abrasion makes wood fibre-reinforced high-density composites an appropriate choice for usage in areas such as construction, automotive, interior decoration, and daily life [1, 2]. Nowadays, giant automotive makers like Mercedes Benz, BMW, Toyota and Ford widely use moulded sheets made of fibre mats to produce various components of their automobiles [3].

The damage modes of fibre-reinforced composites are vital constraints in their applications. Various damage modes have a significant effect on the behaviour and performance of these materials. Moreover, composites developed with natural fibres and matrix materials are mostly orthotropic and predicting their failure is even more difficult [4]. In spite of their distinctive assembly and appearance, adhesively bonded wood products such as Oriented strand board (OSB), plywood, and engineered structural lumber can be distinguished by their macrostructure as wood or adhesive.

In this work, a numerical method is used to evaluate the effect of micromechanical damage modes on the properties' degradation of wood fibre-reinforced composites. The cohesive zone model (CZM) and extended finite element method (XFEM) are used to study the effects of initiation and propagation of fibre-matrix debonding and matrix cracking in various RVEs (Representative Volume Elements).

Firstly, the damage behaviour of these RVEs is studied and the method is validated, then the mentioned method is used to evaluate the properties' degradation of these materials. The obtained results could be used to investigate the properties degradation of natural composite laminates in continuum damage mechanics.

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Analysis of the plane elasticity assumptions and the use of plasticity coupled with damage for the micro-scale analysis of composite materials

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Micro-mechanical analysis has its roots in the analysis of a single fibre embedded in a matrix mainly under transverse tensile loading. This problem has been extensively studied; using analytical models, experimental studies and later on, using numerical tools such as the Finite Element Method and the Boundary Element Method.

According to the experimental results in [1, 2], fibre debonding due to transverse tensile load is a 3D phenomenon that starts at the free surfaces in the locations of maximum normal tensile stress. Martyniuk et. al [1] state that interface debonding and crack kinking both start at the free surface and then progress into the specimen's volume. In contrast to the main conclusions of [1, 2], the trend in numerical and analytical studies on a single fibre embedded in a matrix is to use a 2D plane-strain assumption. The main contradiction comes from the fact that most studies that consider plane-strain always compare the results with in-situ observations in SEM, which are observations on the free surface where the stress state is closer to plane-stress. Only a few authors consider the 3D effects of interface damage under transverse loads, and no publication was found to study the 3D initiation and progression of kinking. This is one of the main knowledge gaps within this type of analysis, there is not a deep understanding of the role of the stress concentration of the free surface on the debonding and kinking and the way this could affect the measurement and approximation of interface strength, interface fracture toughness, potential plasticity effects in the matrix and micro-scale strength of the matrix.

The present work gives a detailed analysis of the consequences of plane elasticity assumptions on the study of failure initiation and propagation in single-fibre models under transverse loading. The present investigation uses cohesive damage to model interface damage and Phase-Field fracture to account for damage inside the polymer matrix. This work focuses on two main aspects, the influence of the out-of-plane thickness of the model and the differences between linear elasticity and pressure-dependent/independent plasticity models. It is found that if a 3D model is used there is a minimum required thickness in order to obtain representative results, these dimensions are controlled by the fibre diameter and interface properties mainly. On the other hand, it is found that linear elastic and plastic behaviour assumptions are affected in different proportions when the modelling approach moves from plane-stress to plane-strain-dominated conditions. In particular, pressure-dependent plasticity models combined with a plane-strain condition may result in unrealistic underestimations of the composite strength.

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Phase field fracture modelling of 3d printed materials: an anisotropic analysis

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Additive Manufacturing is a technology which is more and more consolidated in both industry and academia for the chances that it offers. Among all the fields of application, the one regarding continuous Fibre deposition is among the most interesting since it allows the tailored reinforcement of regions which would be naturally subjected to stress concentrations. The possibility to know in advance the failure pattern of such 3D printed structure is of utmost importance in the design phase, which would need necessarily an experimental verification of the component realized in case no numerical simulations were available. On the other side, being the crack path that could originate from such geometry complex, an adequate numerical tool able to describe complex phenomena like crack nucleation, propagation, branching and coalescence is needed. In this sense, in this work the Phase Field approach to fracture is adopted. To study the ability of Phase Field to correctly predict the crack pattern and mechanical behavior, several numerical examples are taken into consideration, ranging from unidirectional notched specimens to variable stiffness ones, highlighting the validity of the approach.

Different numerical simulations are performed. In the first part of the work, the experimental evidence for unidirectional reinforced notched specimen and an Open Hole Tension specimen is replicated, finding good results both for crack pattern and mechanical response. In a second part, the approach is extended to variable stiffness composites, studying the influence the reinforcement has on the size effect. It is shown that the bigger the specimen, the larger is the beneficial effect resulting by the 'tailored deposition' of the continuous fibre in the variable stiffness specimens compared to the unidirectional ones, as shown in Figure 1.

The work underlines the capability of Phase Filed to predict the fracture behavior in such a complicated scenario like the one of continuous fibre deposition 3D printing. Therefore, the analysis presented here can be used as a general tool for the design of such components, leading the way to an application of composite 3D printing in industrial sectors.

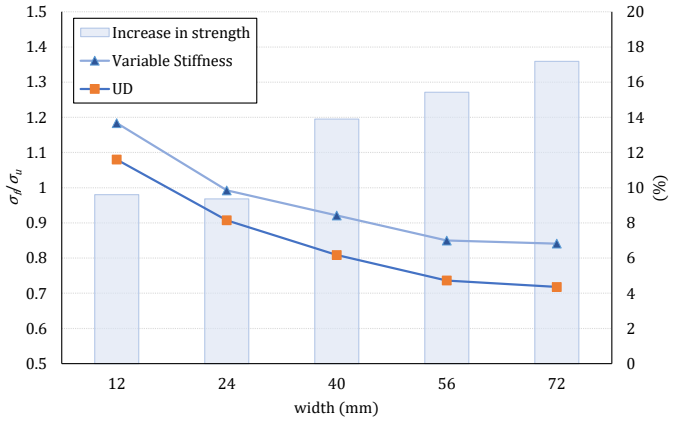

Figure 1 Size effect for the variable stiffness composite and improvement with respect to the unidirectional case.

Rapid crack development in glass modelled by phase field damage approach

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This contribution concerns the response of the laminated glass plates to dynamic loading. Laminated glass is a composite layered material composed of several plies of float glass and polymer interlayers. Although glass is almost purely elastic material before the breakage, it suffers from brittle failure and cracks are developing with a very small process zone. Furthermore, the visco-elastic nature of the polymer interlayer also affects the cracks evolution. As a result it is possible to effectively simulate such material before failure but the initialisation and development of cracks still brings many research challenges.

Simulation of the dynamic response of laminated glass loaded by an external impactor or explosive blast brings several phenomena that need to be investigated:

- Fragmentation and numerous branching that occurs in glass layers
- Contact problem characterises the transfer of the impactor's energy to the laminated plate
- Damping and energy dissipation through rate-dependent viscous interlayer

For brittle material, such as the glass, the phase field damage model appears to be a suitable model. At the very least, it is worth examining it and finding out what can be expected from such an approach. The presented phase-field damage model is based on the assumption that the sharp crack, traditionally represented as a singularity, can be mathematically regularised and spread to a finite length. The position of the crack is obtained by energy minimisation. This brings the the main advantage: the variational approach allows for the initialisation and development of cracks without additional ad hoc criteria.

We are therefore trying to test the aforementioned phase-field damage model for prediction and qualitative assessment of suitability for rapid crack propagation under impact or explosive blast, with a specific application to the laminated glass. We especially want to grasp the damage model itself and use our own code, for that reason the problem is simplified by neglecting viscous effects and solving the contact problem in simplified fashion. The situation is further simplified by using a spatially reduced Mindlin plate model, which significantly reduced the computational demand. The proposed model assumes that the cracks initiate on glass surface. This assumption is considered in the spatially reduced model by the damage initialisation driven by the highest tensile stress near glass surface. With this assumption the resulting crack patterns qualitatively correspond with the experimental results.

Considering simplicity and good agreement to experimental observations, the spatially reduced phase-field damage model proves to be applicable to structural elements made of laminated glass.

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Phase field model for transverse cracks in composites: Effect of residual stresses

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Residual stresses in fiber reinforced composites are inherent due to various factors such as: laminate layup, difference in the coefficients of thermal expansions in fiber and matrix directions, curing cycles etc. This work considers the contribution of all these factors to evaluate the influence of residual stresses on the material behavior in flat and curved composite laminates with 0º/90º cross-ply layup configurations. This behavior is further introduced into the phase field formulation to model transverse cracks in composite laminates, considering both material and fracture behavior.

At first, isotropic phase field formulation in terms of HETVAL subroutine available from the literature [1] is fully exploited by recreating benchmark problems with flat and curved geometries in Abaqus. After establishing a clear understanding of the isotropic model for all the three different formulations AT1, AT2 and PF-CZM, orthotropic material behavior is introduced. Regarding the fracture behavior, various strain energy decomposition methods from the literature are analyzed and the energy split scheme with stiffness degradation method employed in [2] is implemented with only one phase field variable addressing transverse damage. The phase field implementation is further validated by testing the standard models from the literature.

Additionally, the effect of residual stresses, in respect of thermal strains is constituted into the phase field formulation in the straightforward way. The formulation is further validated by performing tests on a flat laminate with 0º/90º layup and corelating the results with the experimental data from [3].

Furthermore, four point bending tests(4PBT) on the $[0,90_2,0_n]_S$ cross-ply curved laminates is conducted to study the induced unfolding failure, a phenomenon where damage is initially initiated by intralaminar matrix crack and propagates further as interlaminar delamination under the presence of high stresses[4]. The detailed finite element study on 4PBT is conducted to assess the following:

1. Induced unfolding failure phenomenon (Stacking sequence is particularly chosen to illustrate the existence of induced unfolding)
2. Comparison with the experimental data [4]
3. Results with and without the effect of residual stresses for AT1, AT2 and PF-CZM formulations to show the significant influence of residual stresses.

To this end, efforts are made to extend this study to curved laminates with quasi-isotropic layups.

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Phase field modeling on the multi-physical damage of composites

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The understanding of water penetration, diffusion, and swelling-related strength degradation is critical for assessing the durability of polymer-based composite materials exposed to marine environment. When moisture intrusion and various external loads are concurrently applied to polymer matrix materials, the multi-physical diffusion process, and the correlation with the complex cracking phenomenon is far from been discovered.

To approach this uncertainty, we explored fully coupled moisture diffusion, stress redistribution, and damage evolution of composites for revealing complex failure patterns and rules. A thermodynamically consistent moisture diffusion model is established to couple the moisture diffusion and viscoelastic response of the multiphase material. A two-constituent phase-field fracture model is developed to describe the hygroscopic swelling in the matrix and interfacial decohesion within a concise and universal continuum mechanics framework. We also propose a crack filter theory to characterize the fluctuation of moisture flux along with the evolution of regularized crack.

We showcased the capability of the model and derived two critical processes related to fundamental physical insights into moisture damage. Moisture diffusion is predicted to accelerate at the interface and vicinity of crack tips with distinct reasons. The moisture diffusion around the fiber/matrix interface is accelerated by the additional moisture gradient generated by the fiber and matrix. The moisture diffusion around the crack tip was accelerated by the hydrostatic stress gradient introduced by the crack. When the moisture-containing composite was subjected to an external load, the hydrostatic stress inside the material increases. Then, the moisture was attracted to the area with a higher positive hydrostatic stress (i.e., the crack tip) and accelerate the inversible material degradation in this area. Thus, a reasonable inference is that the moisture re-diffusion, dominated by the external load, increases the likelihood of failure of the region that tends to fail owing to stress concentration. This inference would be applicable to the other chemo-mechanical coupled problems.

We further revealed the effects of hydro-damage on the mechanical behavior during moisture-induced aging. With multipoint damage caused by moisture diffusion, the crack profiles of composites are predicted to be distinct with dry system subject to tensile loading, which are highly consistent with experiments. Within hydro-composites, the main crack gradually forms according to the coalescence of multiple damage points and tends to nucleate near the diffusion boundary. For dry composites, the main crack tended to appear near the mid-thickness and propagated from a single nucleation point. Generally, increasing these factors will aggravate the moisture-damage (i.e., interfacial decohesion) owing to the increased discrepancy in displacement between the fiber and matrix. This work might provide a new insights into the coupled damage mechanism of polymer composites and facilitating microstructure design to enhance its performance in ocean environments.

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Multiscale analysis of fracture in short glass fiber reinforced polymers through phase field

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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 [6] 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 behavior, the well established isotropic phase field models of brittle fracture [5, 4] is extended towards the anisotropic case making use of the fiber orientation interpolation concept [3].To create the database, the anisotropic elastic coefficients are obtained from previously executed micromechanical simulations on realistic microstructures [6] 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 [2] or from injection moulding process simulation is mapped into the Abaqus mesh prior the execution of the macroscopic simulaiton. The performance of the simulation method is demonstrated by means of several numerical analyses and the predicion 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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An efficient phase field implementation of fracture analysis of functionally graded materials

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Innovative materials known as functionally gradient materials (FGM) exhibit gradual spatial changes in their properties. However, compared to homogeneous materials, FGMs' fracture behaviors are more complex due to graded distributions of their material properties, which makes modeling their failure process extremely difficult. Phase field approaches [1] completely avoid the necessity for monitoring discontinuities explicitly in the domain and the remeshing process, in contrast to other numerical methods like the extended finite element method (XFEM). Low computing efficiency, however, continues to be a problem for the phase-field model's numerical simulation [2], especially in FGMs where material properties are to be evaluated at the integration point level.

The current work makes use of special shape functions and informed mesh refinement schemes to render the fracture computations faster at the same time retaining accuracy in the prediction. To this end, exponential shape finite element shape functions [3] are introduced instead of standard bilinear shape functions conventionally used in finite element calculations. Bilinear shape functions offer a linear interpolation of solution variables inside an element and require closely spaced refined meshes to accurately resolve sharp gradients. Sharp gradients of solution variables are expected along the crack propagation path itself. On the other hand, exponential shape finite element shape functions allow sharp changes of solution variables inside elements. This exponential characteristic can be made use of in reducing the mesh refinement level at crack propagation paths. Although exponential finite element shape functions can be very useful, they offer good approximations only when the shape functions are oriented concerning the crack propagation path [4]. This study suggests a learned orientation scheme for these shape functions, informed by an approximate analysis using bilinear shape functions carried out during the analysis itself. Functionally graded materials, in the interest of fracture predictions, have variations in stiffness, fracture resistance, and Poisson's ratio dependent on special coordinates. A homogenization strategy can be used to infer this from the spatial variation of the volume fractions of the constituent materials. Fracture simulations are carried out in functionally graded plates with different gradation schemes, and their effect on fracture resistance is investigated. Computational efforts incurred in the present implementation are compared with existing schemes using bilinear shape functions.

Several pragmatic examples are considered that show the effect of a material gradient, crack location, and the resulting mode mixity. The results obtained provide fundamental and quantitative insight into the role of the material property gradation on the crack propagation response. The ability of the phase field model in conjunction with exponential finite element shape functions to predict complex crack patterns is proven.

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Finite fracture mechanics: Models and applications

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

New insight into crack front segmentation into facets under mixed mode I+III loading: the role of T-stress and mode-dependent fracture properties

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Crack growth under combined mode I+III loading has been widely studied over the past decades since the pioneering works of Sommer [1] and Knauss [2]. Such a loading leads to a crack rotation around the direction of propagation in order to reduce mode III and reach a pure mode I situation, which is achieved by a fragmentation of the initial crack into multiple daughter cracks usually called facets. Once initiated, some of these facets grow and coalesce to form a stepped fracture surface becoming coarser as the crack grows. Several models such as e.g., [3], are able to capture the crack rotation from a macroscopic point of view. However, modelling the crack front segmentation into multiple daughter crack is still challenging. We previously proposed a model to study crack front segmentation into facets under mode I+III [4] based on a 3D application of the coupled criterion [5]. This model enabled crack initiation shape, orientation and spacing to be determined for any mode mixity ratio based on 3D finite element modelling of a periodic network of facets ahead of the parent crack. While the facet orientation and shape were determined based on a stress criterion, the initiation loading and facet spacing was obtained by coupling both stress and energy criteria. The proposed model is herein refined by considering both the influence of T-stress (parallel to the initial crack front) and mode dependent fracture properties. We show that considering exclusively either T-stress or mode dependent properties, facet nucleation may be more favourable than straight crack propagation but in conditions that are incompatible with experimental observations. It is only by coupling mode-dependent fracture properties and T-stress that it is possible to determine configurations compatible with experimental observations for which facet nucleation is more likely to occur than straight crack propagation. These configurations depend on the critical shear energy release rate and T-stress magnitude. We thus conclude that crack front segmentation into facets is loading and material dependent phenomenon that is not solely related to a mode mixity threshold but also to shear critical energy release rate and T-stress magnitude

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Crack impinging a curved weak interface: Competition between deflection and penetration

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Weak interfaces are able to deviate and arrest the crack progression. Moreover, if the weak interface is not straigth but curve, the effect of crack arrest can be modulated and reinforced, see experiments by [1]. In fact, many natural systems are characterized by the presence of interfaces with non-planar profiles, including textured definitions or wavy patterns which can be accordingly engineered to achieve outstanding fracture response. Thus, curved weak interfaces present promising advantages to be implemented as crack arrestors in structures designed under the tolerant-design principles. Among other advantages, they neither add extra weight nor affect significantly to the global stiffness of the structural element, in contrast with other crack arrestors.

To be employed as crack arrestor, it is key that the interface can deviate the crack. If the crack penetrates across the interface, the effect of the weak interface as crack arrestor is canceled. In view of this, this work studies how to set the interface parameters to promote the crack deviation along the interface. In particular, following the dimensional analysis of the problem, the effect of three significant dimensionless parameters is studied: interface to bulk fracture toughness, interface to bulk tensile strength and the interface curvature radius normalized with the material characteristic length.

The study is carried out using the Coupled Criterion of the Finite Fracture Mechanics [3, 2]. This criterion is able to predict successfully the competition between crack deflection and competition at curved weak interfaces.

The results show that:

- The ratio of interface to bulk fracture toughness is the most relevant dimensionless parameter to switch from crack penetration to deflection.
- The dimensionless radius of the curved interface affects also significantly the failure mechanism governing the deflection/penetration competition.
- The other dimensionless parameters extracted from the dimensional analysis affects much less the competition.

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Finite Element implementation of the Coupled Criterion based on the Principle of Minimum Total Energy subjected to a Stress Condition to predict crack onset and growth

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In the framework of Finite Fracture Mechanics (FFM), Leguillon introduced the coupled criterion of the FFM (CCFFM) [1], which is the base of this work. According to CCFFM, the stress and energy criteria are two necessary conditions to allow an abrupt onset of a crack in a finite extension. A new formulation of the CCFFM based on the principle of minimal total energy subjected to a stress condition (PMTE-SC), suitable for solving complex fracture problems, was introduced by Mantic [2]. This is primarily due to the fact that it is better suited for a generic computational implementation of a load-stepping technique that addresses issues with the initiation and propagation of multiple cracks. In addition, the total energy can be expressed as a separately convex function in the displacements and the damage variable fields. This makes it possible to apply optimisation techniques that are both efficient and stable to achieve the objective of minimising the total energy with constraints.

For implementing PMTE-SC in FEM code ABAQUS, we use UINTER, a subroutine used to define the interaction between two surfaces. It is called at points on the slave surface of a contact pair with a user-defined constitutive model describing the interaction between the surfaces. Here, the interaction between the cracked surfaces is modelled by a continuous distribution of springs with a linear elastic behaviour, Linear Elastic Spring-Surface Interaction (LES-SI). Therefore, the springs interact with the two surfaces of the crack, which act linearly during tension and shear. The mixed mode constitutive law of the active surface springs was described, e.g., by Mantic et al. [3]. The change of the potential energy of the system is calculated by the code using the incremental virtual crack closure technique (VCCT), as it provides accurate results. It is based on the idea that the change in potential elastic energy due to specific crack growth is identical to the work necessary to close the crack with an equivalent extension. In the context of finite fracture mechanics, this idea is applied from an incremental perspective. Several fundamental problems for crack onsite and propagation under quasistatic load in mode I, such as a circular hole in an infinite plate under remote tensile load and biaxial load, rhombus hole specimens under compression, and others in mixed mode, are solved. Therefore, this method opens new possibilities for studying the onset and propagation of cracks.

In this work, a new method to characterise the crack onset and propagation has been developed based on the Coupled Criterion of Finite Fracture Mechanics (CCFFM). This method predicts an instantaneous crack onset or propagation without requiring an infinitesimal crack growth. This allows the appearance of several fractures simultaneously in the same problem. A computational algorithm based on the new formulation, i.e., PMTE-SC, has been implemented using the Finite Element Method in ABAQUS and Python scripts.

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A new computational procedure for singularity analysis of interface cracks with frictional contact in anisotropic bimaterials

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For the study of interface cracks in bimaterials, we must go back to 1959 when Williams [1] introduced an asymptotic analysis of elastic fields at the tip of an interface crack. This model is known as the open model of the interface crack and its solution leads to oscillatory displacement and stress fields around the crack tip. These oscillations in the displacement field imply that interpenetrations between materials near the interface crack tip may occur [2]. To solve this physical inconsistency Comninou [3] proposed the frictionless *contact model for interface* cracks in isotropic bimaterials. Later on, Comninou [4] generalized her model considering frictional contact between crack faces coming to the conclusion that friction makes the singularity weaker, i.e. $\lambda>0.5$.

In this work a generalization of the Comninou contact model of interface cracks to linear elastic anisotropic bimaterials considering the Coulomb isotropic friction law is developed, based on the Stroh formalism [5, 6] and using the concept of bimaterial matrix by Hwu [7]. The present semi-analytic procedure computes the singularity exponents λ that define the asymptotic stress and displacement fields at the interface crack tip. Unlike several previous approaches found in literature, this work does not impose a direction of sliding between both materials, considering the sliding angle ω as an unknown. Once the singularity exponents λ and corresponding sliding angles ω are computed, the displacement and stress fields at the crack tip associated with each singular mode can be obtained. After analyzing the displacement and stress fields in the frictional sliding interface, it is concluded that, as Comninou [4] pointed out for isotropic bimaterials, in the case of monoclinic materials with a symmetry plane $x_2 = 0$, that is, any stacking of layers in a composite laminate, friction also weakens the friction interface crack tip singularity.

One advantage of the developed methodology is that, despite using the Stroh formulation for mathematically non-degenerate anisotropic materials, the final expressions of the two nonlinear eigenequations depend on the bimaterial matrix, which can be expressed in terms of the real Barnett-Lothe [8] tensors, **H**, **L** and **S**. This allows a direct application of the present methodology to isotropic and transversely isotropic materials.

The weak singularity allows the use of the crack tip solutions computed by the present methodology to predict the growth of such interface cracks by the Coupled Criterion (CC) [9] of Finite Fracture Mechanics (FFM) as proposed by García and Leguillon [10] and Graciani and Mantič [11].

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Failure of notched zirconia specimens under residual stress

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When machining zirconia (Y-TZP) notched samples, honing of the notch causes a phase change from a tetragonal to a monoclinic micro-structure [1] along the surface. The result is a thin layer where a strong compression prevails, up to 1.8 GPa and linearly decreasing in depth until 7–8 µm. Moreover, these residual stresses depend also on the notch root radius ρ, which is one variable parameter of the experiments. They reach a maximum for ρ between 5 and 12 µm. For wider notches with radii above ~ 90µm created by cooled diamond grinding they are significantly smaller [2]. When testing the specimens in 4-point bending, this obviously leads to an apparent increase in strength and toughness.

Experiments were carried out on various specimens with ρ varying from 6 to 90 µm. Two types of specimens were tested, one as sintered and the other having undergone a heat treatment in order to release the residual stresses (heating at 1100 °C for 1/2 hour).

We propose in this work to use the Coupled Criterion (CC) [3,4] to predict this apparent enhancement of the fracture properties and compare with the experiments. Indeed, the CC is twofold, it requires to verify an energy condition, as does Griffith's criterion, but also a stress condition which must be very sensitive to the presence of high residual stresses. Moreover, it does not require the modeling of a prior defect whose dimension could be chosen more or less arbitrarily.

Calculating the residual stresses and solving the elastic problem of bending are carried out separately by Finite Elements and then combined. This separation is made mandatory because of the different boundary conditions in the two problems. Residual stresses due to honing or grinding are obtained using a similarity to thermal residual stresses. A first scalar field is built along the notch surface, taking the value 1 at the surface and linearly decreasing to 0 at a distance of 7 µm. It can be associated with the volume fraction of monoclinic phase and will be used, by analogy, as the temperature field. It is subsequently calibrated so that the compressive residual stress takes the value 1.8 GPa at the surface as reported in [1]. On the other hand the simulation of the 4-point bending loading is standard.

The stress field is first computed on the uncracked structure along the expected crack path (the symmetry axis). Then, a virtual crack of variable length is created by unbuttoning pairs of nodes. For each length, the strain energy is computed, allowing to define the energy function involved in the CC as a function of the crack length. The implementation of the CC amounts to solving two inequalities that provide the critical load causing the failure and the crack length at initiation.

Despite the thinness of the residual stress zone, the comparison with the two cases, thermally treated or not, is conclusive. The CC captures the apparent improvement in the fracture properties of the material in a very satisfactory way.

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FEM implementation of the minimization of the total energy subjected to a stress condition to predict delaminations in ILTS tests

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Inter-Laminar Tensile Strength (ILTS) test uses L-shaped composite coupons with laminas having different orientations. In the present investigation, this mechanism is modelled using a quite general formulation of the Coupled Criterion of Finite Fracture Mechanics (CCFFM) [1] applied to the Lineal Elastic Brittle Interface Model [2] (CCFFM + LEBIM) [3] based on the Principle of Minimum Total Energy subjected to a Stress Condition (PMTE-SC) [4].

The PMTE-SC, employing a load-stepping procedure, minimizes the total energy functional, the sum of the potential and dissipated energies, in the feasible region of all possible new crack configurations given by the stress criterion, in each load step. A great advantage of PMTE-SC is that the total energy is separately convex in displacements and damage variable. This feature allows solving convex optimization problems separately in terms of displacements and damage variable in each load step, which makes this procedure very robust and efficient especially if a suitable staggered scheme of minimization is applied. In the literature similar staggered schemes are also referred to as Alternate Minimization Algorithm (AMA) [5]. The PMTE-SC with a suitably modified AMA has been implemented in a Python script using the commercial FEM code Abaqus.

In the ILTS test, a four-point bending test tool applies a purely bending load to the curved part of the specimen. For this purpose, the test includes four freely rotating rollers in contact with the specimen.

In these tests, microcracks appear first, which after their coalescence produce intralaminar failure. This failure propagates in an instable manner in the form of delaminations, this type of instability is known as snapback. In fact, almost instantaneous delaminations occur at the remaining interfaces, so it is not trivial to determine the point or points at which failure initiates. To capture this unstable appearance of the damage, the experimental test should allow the simultaneous reduction of the load and the displacement. In classical numerical simulations, this behavior manifests itself in the form of convergence problems due to sources of model nonlinearities, thus the use of a robust numerical tool is needed.

Preliminary calculations carried out by means of the code implementing PMTE-SC with the modified AMA have shown that this code is an adequate tool to predict onset of multiple delaminations in the ILTS specimens.

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Modelling of glass matrix composites by the Coupled Criterion and the Matched Asymptotic Approach. The effect of residual stresses and the volume fraction.

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Ceramic platelets are used as a reinforcing constituent in glass matrices to improve mechanical properties such as the fracture toughness [1]. One example is the borosilicate glass Al_2O_3 platelet composite, an interesting material for industrial applications due to its low production cost and environmental safety.

One of the most important characteristics of this composite material is the thermal expansion mismatch between glass and alumina [2]. The latter has a higher thermal coefficient than the one in glass, and consequently, compressive and tensile residual stresses will appear after cooling in the matrix and the platelet, respectively. These residual stresses have been studied experimentally [2] and numerically [3].

In [4], a new methodology to design and study platelet composite was presented, based on the application of the Coupled Criterion (CC) [5] together with the Matched Asymptotic Expansion (MAE) [6]. The tool studied only the role of a single platelet, without including residual stresses. Thus, the objective of this work is to complete the numerical method introduced in [4] including the influence of the volume fraction and the thermal mismatch mentioned above. The model is validated by comparison with experimental results found in the literature.

The improvement of fracture toughness is related to a change in the path of a pre-existing crack assumed in the specimen, under the presence of a platelet with a certain orientation. Two cases are studied, when the platelet is parallel to the pre-existing crack and when it is perpendicular. In the latter the predominant mechanism is determined among different possibilities: a penetration of the crack in the platelet, a deviation through the interface glass/alumina, a decohesion of the lateral face of the platelet or a crack jump into the glass. Results are shown at the scale of experiments [1] and at different scales, in order to study the platelet size effect on the composite fracture toughness.

Therefore, a complete design tool for this kind of composites is presented, particularized for the case of a glass matrix reinforced by alumina platelets. The key novelty of this methodology is the possibility to study separately different factors that contribute to the improvement of the fracture toughness: geometrical factors, such as the volume fraction, the size and the orientation of the platelet, or environmental factors, in particular the effect of residual stresses. Furthermore, this design tool seems to have an important reduction in the computational complexity with respect to other analysis found in the literature. The method can be used to optimize the design of platelet composites.

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A Model Based on Finite Fracture Mechanics to Predict the Fatigue Lifetime of Notched Components

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This study presents a model based on Finite Fracture Mechanics (FFM) [1,2] to predict the fatigue lifetime of notched structures under uniaxial loading. The investigation focuses on the medium/high-cycle fatigue regime and assumes that stage II is dominant during the fatigue process, so that a linear elastic mechanics approach can be employed under mode I loading conditions.

The coupled FFM approach is based on a discrete crack extension and on the simultaneous fulfilment of two conditions: a stress requirement and an energy balance. Originally proposed in the static framework [1,2], the criterion was later extended to the fatigue limit regime [3,4]. To describe the brittle failure behavior of notched components, FFM implements two material properties: the ultimate tensile stress and the fracture toughness for static loadings; the high-cycle fatigue strength as well as the threshold value of the stress intensity factor (SIF) range for cyclical loadings.

To develop FFM for estimating finite fatigue life, a new couple of material properties called critical cyclic stress and SIF at failure are introduced. Moreover, it is supposed that they follow a power law relation with respect to the number of cycles (Basquin's equation).

To determine the variation of critical cyclic stress, a best-fitting interpolation procedure is applied to experimental data obtained from plain samples. On the other hand, to estimate SIF at failure, an inverse calibration of Basquin's equation is performed on experimental data related to notched samples. FFM reverts to a system of two equations in two unknowns: the number of cycles to failure and the critical crack advance.

Finally, the FFM model is validated using experimental results of samples weakened by V-notches, U-notches or circular holes made of EN3B steel [5]. Tests were performed under tension-compression or tension-tension loading and different loading ratios. The number of cycles to failure was determined by 50% decrease in initial stiffness. The results from the tension-compression loading case show that the FFM predictions for different samples are satisfactory, falling within the scatter band 1/3 and 3. For the tension-tension loading, , the finite life predictions agree with the experimental data, but are more conservative for bending samples. The present approach thus reveals promising for lifetime estimations of notched components and allows to overcome the drawbacks related to approaches based on critical distance which reveals a material property.

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Finite Fracture Mechanics versus Phase Field models of fracture: A case study on the crack onset from circular holes under biaxial loadings

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The phenomenon of brittle crack onset stemming from a circular hole embodied in a biaxially loaded infinite plate is herein investigated. Analyses on the dependence of the conditions upon failure with the loading biaxiality reveal a wide casuistry in terms of the sign and trend distributions of both the stress field and energy release rate. This renders the considered case study exhaustive towards assessing different failure criteria. This feature is thus exploited towards conducting a thorough assessment of the crack onset predictions by three different in vogue approaches: Finite Fracture Mechanics, Cohesive Zone Model and Phase Field models of fracture.

Failure predictions by the original formulation of the Finite Fracture Mechanics' coupled criterion [1] result to be consistently more optimistic than those of the averaged-stress counterpart proposed in [2]. Still, both approaches agree to state that there exists some tension-compression and bi-compression loading states for which a certain range of hole sizes are associated to energy-governed failures, with no direct participation of the stress condition. Remarkably, this implies that Finite Fracture Mechanics may foresee failure nucleation as strength-independent for non-singular geometries.

Furthermore, the well-established Dugdale's Cohesive Zone Model [3] is implemented towards providing some benchmark crack onset predictions, which result to be close to those by the Finite Fracture Mechanics approach. In line with what seen in the literature, there is a better agreement with the latter's original formulation, yet to an extent that varies with the loading biaxiality and the hole size.

Lastly, the Phase Field model of fracture is implemented paying special attention to the choice of the strain energy decomposition (in terms of the energetic contributions of tensile and compressive states), being herein implemented two relevant options: No-Decomposition and No-Tension decomposition (see [4]). As expected, the former model yields an utter unrealistic behavior as for being symmetric in tension and compression. On the other hand, the No-Tension choice results a much more accurate option for it restricts failure to tensioned regions. Furthermore, this model yields failure onset predictions in satisfactory agreement with Finite Fracture Mechanics, specially in the cases where the latter's predictions fall in the intersection of stress and energy conditions. As a result, the Phase Field model of fracture using the No-Tension strain energy decomposition is deemed a solid contender for predicting crack onset in scenarios with combined tension-compression stress states along the prospective failure region. Consequently, it is further used to study the interaction between arrayed holes and the resultant crack onset behavior.

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Influence of elastic and fracture anisotropy on architectured materials using coupled criterion and matched asymptotic approach

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Architectured materials are materials for which the structure is configured across the scales in such a way that it exhibits attributes not exhibited by any of the constituents alone [1]. They encompass a large variety of applications, e.g. shock absorption, insulators. Some particular architectures enhance fracture resistance. For instance, 3D-printed-induced polycarbonate architecture can generate anisotropic toughness [2]. Nacre-like alumina (NLA) is composed of stiff alumina platelets along with a glass secondary phase presents at the platelet interfaces. The alumina platelet arrangement over the length scales induces anisotropic elastic and fracture behavior [3]. In both cases, the microstructure anisotropy plays a bivalent role on fracture behavior. On one hand, it induces anisotropy in the elastic and fracture properties, that themselves influence the fracture behavior. On the other hand, microstructure anisotropy can trigger different fracture responses [4]. Consequently, it is possible to play on both aspects to optimize microstructures with respect to toughness. Thus, a finite fracture mechanic implementation of the coupled criterion [5] is used to assess the effect of elastic and fracture parameter anisotropies on crack initiation in a notched homogeneous bending sample.

Then, the effect of elastic and fracture parameter anisotropy on crack propagation is assessed using cohesive zone models. Thus, guidelines to improve the material behavior through elastic and fracture properties optimization with respect to both crack initiation and propagation can be defined. Finally, this approach is applied on a model accounting for NLA microstructure. The effect of platelet dimensions, orientations and distribution on crack initiation and propagation is assessed. Using both a homogenous model and a model accounting for the microstructure allows to differentiate fracture reinforcement caused by solely the microstructure, or the material elastic and fracture parameters.

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Validated model for predicting crack initiation from arbitrary-shaped notches

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In engineering, it is often asked what is the maximum load a component can withstand before it fails. The coupled criterion [1, 2] was introduced to predict the failure from notches accurately. It combines a stress- and an energy-criterion. At a position at which both criteria are fulfilled simultaneously a crack will initiate and failure will occur. One drawback is that the energy-criterion requires the incremental energy release rate which has only an analytical solution for very simple notch geometries like V- and U-notches.

To compute the incremental energy release rate for an arbitrary-shaped notch the Finite Element Method (FEM) can be used. If the failure should be predicted at all positions on a notch, virtual cracks are introduced sequentially all along a notch surface in an FEM model and the incremental energy release rates are computed from the deviation of the strain energies. Since, for each position on the notch several simulations with various crack lengths are performed, this approach is computationally intensive.

The authors developed an efficient two scale approach to apply the coupled criterion all along a notch surface [3]. The larger component scale utilizes a FEM analysis and provides the displacement- and force-field. The local model provides the incremental energy release rate and is parametrized by two dimensionless quantities. This allows to scale the local model and use it for materials of various stiffnesses. The local model is computed in advance for various virtual crack lengths and for five deformation modes that are used to fit the forces and displacements of the component model with the help of linear superposition. Furthermore, the local model approximates the local curvature of the notch by a quadratic function. However, since the local model behaves similar to a submodel with fixed boundary conditions, the energy release rate is underestimated if cracks are introduced. Therefore, automatically weighted force- and displacement-controlled boundary conditions can be used. Those boundary conditions allow a deformation during the opening of virtual cracks. That makes the prediction of the incremental energy release rate more accurate.

Our two-scale approach has the disadvantage that for some geometry and material combinations the initiation length of a crack is longer than the size of the local model. In this case no prediction is possible.

The goal of this work is to define where our approach works and under which circumstances it is essential to use the coupled criterion, because a stress-based criterion gets too inaccurate. Therefore, experimental tensile tests of specimens containing various notches are provided. Furthermore, the maximum load is predicted using a stress-based criterion as well as the coupled criterion.

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Finite Fracture Mechanics: Size effects on spheroidal voids and corrosion pits

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The present work aims at investigating the size effect of a spheroidal cavity in an infinite linear elastic continuum under remote tension, by means of the coupled Finite Fracture Mechanics (FFM) [1] approach. FFM is a coupled fracture criterion which allows to provide strength predictions based on the simultaneous fulfilment of a stress condition and the energy balance. Although initially proposed and applied only to static problems, FFM was later extended to assess the fatigue limit of structural components [2]. Whereas the static formulation requires the knowledge of the material ultimate tensile strength and of the fracture toughness, both the plain fatigue limit and the threshold value of the stress intensity factor range are needed in the fatigue regime.

To implement the FFM, the longitudinal stress field and the Stress Intensity Factor (SIF) related to an annular crack surrounding the spheroidal void, are obtained numerically through a parametric axisymmetric Finite Element Analysis (FEAs). In these analysis, to evaluate the effect of the void geometry, the void axis ratio is varied between 0.1 and 10. Furthermore, to encompass also the influence of the material, different Poisson's ratios are considered ranging between 0.1 and 0.5. Semi-analytical approximating functions providing the stress concentration factor K_t and the SIF itself are put forward.

In the framework of fatigue failure, one of the most important issues is that related to corrosion pitting, a very localized and critical form of damage. Studies focused on this topic have been proposed since the middle of the last century, by approximating the pit shape as in between hemispherical and hemispheroidal. In particular, different works focused on the estimation of K_t, through three-dimensional (3D) FEAs. On the down side, precise 3D FEAs are computationally expensive and thus not adequate for preliminary sizing of structural components. Furthermore, K_t based studies are not able to catch any size-effect according to classical linear elasticity. For these reasons, Härkegård (2015) [3] approximated the fatigue behaviour of a hemispherical pit by that of a spherical cavity in an infinite tensile body. Following this idea, in the present study, the strength estimations, obtained for a spheroidal void in an infinite linear elastic continuum under remote tension, are compared with experimental fatigue data related to corrosion pitting on two different material: (i) 12% Cr martensitic [4] and (ii) 17-4PH turbine-grade steels [5].

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Minisymposium MSA:

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A multiscale phase field fracture approach for rubber-like materials

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In recent years, the phase field method has developed rapidly for modeling fracture in various materials, including concrete, steel, biological tissues, and rubber-like materials. This method approximates cracks by a smooth auxiliary scalar field and has proven to be effective in simulating complex fracture phenomena such as crack nucleation, propagation, branching, and merging. In the case of rubber-like materials, modeling their fracture behavior is crucial for understanding and designing against failures in fields like stretchable electronics, self-actuators, and implantable sensors. However, there exist several challenges when adopting the phase field fracture approach to highly deforming materials like rubber.

Firstly, accurately capturing the fracture behavior in these materials is hindered by their incompressible behavior, which can cause numerical instabilities. To address this issue, a multiscale polymer model is coupled with the phase field approach and formulated using mixed elements to capture the fracture behavior in incompressible rubber-like materials. At the microscale, non-Gaussian statistics is used to model the chain behavior, while the phase field approach is used to model the damage caused by the failure of chain segments. A 3-field mixed formulation is employed for numerical stability, and the incompressibility constraint is enforced in the undamaged regions using augmented Lagrangian iterations. The model's performance is validated by comparing the simulation results with experimental data.

Secondly, although there are many micromechanically motivated models for capturing their failure characteristics, many utilize network models which predict an isotropic network response for bridging deformations at the two scales. However, they may not effectively capture effects on the fracture behavior of microscale phenomena like strain-induced crystallization, which have been found to produce anisotropy in the network behavior [1, 2]. Therefore, in this study, a multiscale polymer model, which is bridged using the maximal advance path constraint [3] network model, is coupled with the phase field approach for modeling crack propagation in elastomers. At the microscale, non-Gaussian statistics is utilized for modeling the chain behavior while accounting for the internal energy due to molecular bond distortions. The non-affine maximal advance path constraint network model, modified for damaged systems [4], is utilized to bridge the deformations at the two scales. The phase field approach is used for modeling the damage, which is assumed to be caused mainly due to the failure of chain segments. Using micromorphic regularization, dual local-global damage variables are introduced and connected using the augmented Lagrangian method. The performance of the model is validated by comparing the simulation results with experimental data.

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Multi-scale fracture mechanics using the FEM^2/IGA^2 method

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In this contribution, we present a multi-scale fracture framework, allowing us to consider individual fracture behaviour on multiple scales. We utilize the well-known FEM^2/IGA^2-method for macroscopically modeling complex materials with heterogeneities on the micro-scale, see Schmidt et al. [1]. In this talk we address additionally the established phase-field method for fracture mechanics, see Hesch et al. [2].

To be specific, we apply the macroscopic deformation at a given point to a representative volume element via suitable boundary conditions and superimpose the macro-phasefield in this point onto the micro-phasefield of the $\mathcal{RVE}$. Introdcing a suitable homogenization technique including different fracture dissipations on the micro- and macro-scale, we obtain an energy preserving formulation. Moreover, we are able to derive consistent linearization of macroscopic stresses, the phase-field driving force and multi-field contributions for the Newton-Raphson iteration.

For the presented framework, we demonstrate its behaviour and accuracy applying a variety of benchmarks, e.g. two-dimensional fracture mode tests for the macro-scale. We investigate different crack growth behaviours, from pure micro- or macro-fracture to combined and accumulated fracture.

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An efficient pcg based multigrid strategy for crack propagation simulations in heterogeneous materials using 3D images: material properties and interface effects

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Numerical modeling of fracture is one of the most powerful ways to let researchers understand and predict failure of cracked structures. The phase field modeling is a widely used computational fracture model due to numbers of advantages. However, performing 3D phase field modeling with real μ-structures is still expensive and complicated due to numbers of challenges, *e.g.* memory requirement, mesh complexity [1].

Based on our previous work on image-based simulations for thermal and mechanical problems [2, 3]. A matrix-free type preconditioned conjugate gradient solver based multigrid method was proposed in our work [4] to perform the phase field modeling. With the strategy developed in [4], we can automatically and efficiently perform the 3D phase field modeling of fracture at the microscopic scale using CT images without making geometrical hypothesis.

In this talk, we will present our recent results obtained on considering the presence of the interface between different materials, during the crack propagation simulations, using the efficient strategy developed in [4]. The micro-macro interactions are also demonstrated by studying the influences of materials properties at the microscopic scales. The importance to consider the presence of interfaces is approved by the good agreement found between the simulation and the experiment.

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A multiscale and multi-physics boundary integral model for polycrystalline materials including damage initiation and evolution under different loading scenarios

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Polycrystalline materials, either metals, ceramics or alloys are ubiquitous all sectors of engineering. The macroscopic properties of polycrystalline components, including the initiation and evolution of damage and its transition from the microstructural level – the *material* scale – to the macrostructural level – the *component* scale – depend on the morphological and constitutive features of the crystals and their intergranular interfaces.

Thanks to the remarkable momentum gained by experimental materials nano/micro-characterisation on one side and high performance computing (HPC) on the other side, the last few decades have witnessed the tremendous development of the paradigms of *multi-scale materials modelling* and *materials by design* [1], where the emerged experimental and computational capabilities are combined in the attempt to understand and explain complex hierarchical material behaviours first and to employ the gained knowledge to design novel materials, through the fine control of their micro-structure, then.

Despite the wider affordability of HPC, fully 3D multiscale computations remain a daunting task, especially when highly non-linear phenomena, such as initiation and evolution of damage, phase changes, etc. are considered. For such a reason, the development of computationally effective, accurate and reliable formulations remain an important task, which complements progress in computing hardware as well as in costly experimental equipment.

In this context, the present contribution reviews the recent development of a computational framework for multiscale analysis of polycrystalline components subject to different loading scenarios and including the evolution of material damage and cracking [2, 3]. The underlying formulation employs generalised Voronoi tessellations for representing the material micro-morphology and boundary integral equations for modelling of the fully anisotropic behaviour of the constituent grains. The initiation and evolution of either inter- or trans-granular damage and cracking is represented through cohesive traction-separation relationships that, by virtue of their mathematical form, are conveniently coupled with the integral equations modelling the behaviour of the individual crystals.

The use of the developed framework for computational homogenization a micro-cracking analysis of polycrystalline aggregates under either monotonic quasi-static loading, low or high cycle fatigue, in presence of hydrogen embrittlement or thermo-mechanical loads is illustrated [4]. It is also shown how the tool can be used for investigating the inter/trans-granular cracking competition and for analysing piezoelectric aggregates. Eventually, the development of a BE^2 framework is described and possible future developments of the presented formulation are discussed.

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2D modeling of compressive failure in recycled aggregate concrete using the mesh fragmentation technique

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The internal structure of concrete is made of different component phases and weak interfaces distributed at the mesoscopic level which are highly related to the complex mechanical behaviors observed in the material. Particularly, the numerical prediction of its compressive failure is a challenging topic involving aspects such as initiation and coalescence of microcracks, dilatancy, localized deformations and degradation [1]. However, a continuum macroscale model that describes more closely such aspects requires a high level of complexity. Therefore, multiscale models equipped with damage or plasticity models have been used to better understand the influence of the distinct phases of the concrete on the fracture process. Such models can be especially useful for recycled aggregate concrete, which presents even more complex meso-structure due to the various components, such as natural aggregates, new and old cement mortars, and several interfacial transition zones.

Therefore, in order to investigate the compressive failure process in recycled aggregate concrete elements, this work employs an extension of the mesh fragmentation technique developed by Manzoli et al. [2]. The material is represented in a mesoscale level, as proposed by Rodrigues et al. [3]. Once the mesh fragmentation technique is applied, interface elements are inserted into the standard finite element mesh to define the potential fracture paths. However, in this study, the interface element type is a two-layer condensed high aspect ratio element. The two layers are respectively ruled by tensile and frictional shear constitutive models, allowing to describe the compressive failure as a combination of both processes, as proposed by Gimenes et al. [1].

Following this approach, the tensile damage model layer enables the representation of fracture propagation in mode I, corresponding to the debonding (opening) between the material elements due to tensile stress. Complementarily, the frictional shear layer represents fracture propagation in mode II, corresponding to the sliding process in the failure surface.

Since the study is mainly focused on the mechanical behavior of recycled aggregate concrete, it is reasonable to assume the mesh fragmentation should be applied to the aggregate elements as well, to account for possible fracture propagation through the recycled aggregates, as observed in experimental findings [4].

In this work, numerical compression tests are carried out in specimens respectively made of mortar, natural aggregate and recycled aggregate modeled concrete. The numerical results obtained are compared qualitatively and quantitatively with experimental results from the literature [4], indicating that the proposed approach is suitable for describing the failure process of natural aggregate concrete (NAC) and recycled aggregate concrete (RAC) in compression. Furthermore, it is observed that the cracking process differs for RAC and NAC, providing better understanding of the participation of each component phase into the composite failure process.

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On the Use of Analytical Homogenization for Modelling of Masonry

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Despite a large number of formulations available in the literature [1], limitations in terms of computational cost, discretization strategy, and calibration effort are still determining factors in the application of numerical models for the analysis of masonry structures.

Brick-to-brick models, where the brick units are used as the basis for the discretization strategy, are associated with heavy computational costs. They are, however, simpler to calibrate than continuous macroscopic models (albeit still difficult), requiring tests to be performed on the interface between brick and mortar and/or on the two constituents themselves.

On the other hand, continuous models at the macro-scale, which treat the material as a homogenous medium, are generally much cheaper to run. However, these models tend to be phenomenological, and therefore very difficult to calibrate: they require multiple destructive tests on large ensembles of bricks, which often cannot be done in practice, particularly when it comes to in-situ assessments of existing structures

Between these two approaches exists a gap in the form of a model which is both possible to calibrate, particularly with limited in-situ testing, and sufficiently cheap to run, potentially applicable to large structures. This is necessary for engineering practice to create full-scale models of existing construction, where masonry is a very typical material for residential and historical buildings as well as infrastructure. An interesting alternative to bridge this gap is the use of homogenization methods.

Homogenization models are based on constitutive formulations at the level of the component materials. Therefore, calibration can often be achieved with small-scale tests, which are suitable for on-site or field-extracted samples. The material behavior is then up-scaled to the macroscopic level, where larger elements can be used for the discretization.

While up-scaling can be done in many different ways, the authors take particular interest in analytical homogenization, as e.g. [2-3]. This approach allows considering phenomena at the constituents' level (brick and mortar), but still limiting computational costs.

The aim of this work is therefore three-fold. First, it contextualizes homogenization-based techniques within the scope of numerical strategies for masonry. While doing so, it also highlights the gap between existing models and material testing limitations, particularly in the case of in-situ and minimally destructive testing. Lastly, it aims at identifying homogenized formulations that can be more easily calibrated and applied to the modeling of existing masonry structures, where the aforementioned limitations play a big role in material characterization.

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The Fully-nonlocal Quasicontinuum Method: A Concurrent Multiscale Approach to Predict Fracture in Periodic 3D Metamaterials

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Given the ongoing up-scaling of manufacturing processes, the prediction of the robustness of the macroscale response of a fabricated structure in the presence of imperfections, e.g., pre-cracks, is crucial. While fracture of linear elastic continua is well-characterized by the toughness K_{IC}, recent studies suggest that this is not necessarily the case for 3D mechanical metamaterials, even in the linear regime [1]. It was shown that the fracture toughness is affected by not only the crack size but also the load triaxiality. They further showed that the effect of the triaxiality and the number of unit cells (UCs) over the crack flank can be captured via a single parameter, which is related to the T-stresses. These observations suggest that the commonly reported metamaterial scaling laws are insufficient to characterize fracture in 3D truss-based metamaterials. To investigate fracture in large manufacturable specimens that contain millions of periodically arranged UCs, continuum finite element simulations are too costly. Therefore, homogenization becomes the method of choice. However, classical hierarchical homogenization techniques rely on the assumption of a separation of scales. When the separation of scales brakes down, e.g., in the case of fracture mechanics, such techniques fail. Therefore, we present a concurrent multiscale technique, viz. a fully-nonlocal quasicontinuum (QC) multi-lattice formulation based on a conforming mesh. Our QC formulation is applied to trusses, whose struts are represented by linear elastic, geometrically nonlinear corotational beams. This setup captures significant nonlinearity and localization effects in fully-resolved regions, while efficiently approximating the remaining simulation domain through a coarse-graining technique. Coarse-graining is achieved by selecting representative UCs (RepUCs) and introducing geometric constraints based on interpolation, here exploiting finite-element interpolation. Previous studies showed that within coarse-grained regions the strain energy of bending-dominated lattices undergoing non-uniform deformation is overpredicted when using affine interpolation. The overprediction was shown to occur due to overconstraining the lattice by preventing bending without stretching of individual truss members [2]. Therefore, we extend the existing framework by introducing higher-order interpolation in the coarse-grained region, while using the simplicity of affine interpolation in the discrete, fully-resolved domain. In conclusion, we present an efficient multiscale framework to investigate fracture in periodic truss-based metamaterials. The method is equivalent to a fully-discrete calculation in certain regions, e.g., near the crack flank, where every UC is also a RepUC, but is significantly more efficient in coarse-grained regions. Results include the fracture toughness of a variety of stretching- and bending-dominated truss lattices.

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A multiscale analysis of dynamic fracture propagation in complex materials

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In recent years, the development of increasingly complex materials has accelerated. To obtain a deeper understanding of the behavior of such materials and the underlying processes numerical simulations can be beneficial. One material, that is focus of current research and a promising new option within the construction sector, is fiber-reinforced concrete. In order to enhance the mechanical properties of traditionally used concretes, short fibers are embedded into a fine-grained concrete matrix. This increases its ductility and tensile strength, making it particularly suited for applications where components are potentially exposed to impact loading.

When considering dynamic loads, a detailed understanding of the considered material is particularly important because of the resulting inertia effects and occurring complex wave reflections. Additionally, designed materials with such an elaborate material composition require the incorporation of microscopic effects onto the overall material behavior. Here, microscopically small cracks develop, which propagate and lead to complex fracture networks through coalescence and branching.

In order to simulate all of these processes, a reliable and efficient multiscale framework must be developed, that includes dynamic effects and can handle localization phenomena. This is achieved by using features of the Multiscale Projection Method [1] and the Generalized Finite Element Method with global-local enrichment [2]. The basic idea is to include microscopic aspects into the coarse scale simulation through an additional, more detailed, fine scale analysis within certain areas of interest. This is accomplished by performing a separate simulation, permitting the incorporation of a different, more accurate, material model, or the explicit representation of fibers and micro cracks. Fine and coarse scale are coupled in a concurrent way: first, the displacements obtained from the coarse scale simulation are enforced as boundary conditions for the fine scale problem. Here the phase-field method for fracture is employed, in order to represent the complex fracture behavior of fiber-reinforced concrete. The displacement field obtained from this simulation is then used to construct a numerical enrichment, that reproduces the displacement jump across cracks on the coarse scale. Moreover, the material degradation resulting from the phase-field formulation on the fine scale is projected back to the coarse scale, in order to account for the loss of stiffness within damaged material.

Since incorporating dynamic effects and fracture into multiscale simulations can be problematic due to spurious wave reflections at domain boundaries and crack surfaces, simplified 1D investigations are conducted. From these studies, conclusions can be drawn on possible modifications of the method, such as an improved enrichment strategy, so that even complex 3D problems with advanced materials, like fiber-reinforced concrete, can be modeled.

With the help of this multiscale method, the simulation of dynamic fracture propagation in complex materials is possible. The influence of underlying micro structural effects is included within restricted areas, while the overall structural analysis is kept simple and efficient.

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Multiscale - atomistic/mesoscopic approach for the determination of fracture criterion in uranium dioxyde - UO_2

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For the thermomechanical modeling of the global evolution of the nuclear fuel (UO_2) during a hypothetical accident situation such as RIA (Reactivity Initiated Accidents) [1], it is necessary to establish a reliable UO_2 grain boundaries fracture threshold, whether it be in terms of stress or energy of the grain boundaries. At present, the fracture thresholds used in nuclear fuel simulation codes need to be consolidated by experience and theory. The aim of this study is to obtain, by calculations at two scales (atomistic/mesoscopic), mechanical and fracture parameters of grain boundaries.

Our approach consists of feeding a mesoscopic model with data from simulations at the atomic scale. The atomistic simulations are of the molecular dynamics type and use a variable charges semi-empirical potential (SMTB-Q [2]) to describe the interactions between atoms. These calculations, carried out using the LAMMPS software, are performed on three grain boundary nanoscale structures representative of UO_2 at different temperatures. The atomistic simulations allow to obtain elastic properties and local fracture parameters (maximum stress and fracture energy) characteristic of the grain boundaries studied.

The results from atomistic calculations are then used as input data in cohesive zone models to perform simulations at the scale of the uranium dioxide grains which is that of the micron. At this scale, cohesive-volumetric approach using the concepts of Frictional Cohesive Zone Model (FCZM) in a multibody systems framework based on the Non-Smooth Contact Dynamics (NSCD) is employed [3]. The impact of the presence of intergranular bubbles of different sizes is studied. A plastic model is used in the volume to consider possible dislocation movement in the system. The associated calculation code, called XPER, allows to analyze cracking induced by grain boundaries. The results are compared with the experiment to validate the approach.

In the end, we propose, based on results of the present study, a failure criterion that can be used in macroscopic simulation codes of nuclear fuel.

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Micro-to-macro mechanical modeling of corrosion-induced cracking

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Corrosion of reinforcement bars in concrete plays a significant role in determining a structure's durability and serviceability lifetime [1]. Chemical species (Fe2+, OH–) diffuse through the pore space of cementitious material and undergo various chemical reactions, which lead to the formation of corrosion products (Fe(OH)2, Fe(OH)3) within the pore space. Over time, these precipitates grow and exert pressure on the solid phase, which leads to fracture initiation and, ultimately, to the deterioration of a structure. In concrete, pore sizes range from nanometers to micrometers with a random spatial distribution. This stochastic nature is expected to influence the ionic diffusion in the pore network and the development of stresses in the matrix. Furthermore, the three mechanisms involved: ionic diffusion, chemical reactions and stress development, are strongly influenced by each other, and their interplay is thus crucial to fracture initiation.

Despite its importance, corrosion-induced cracking has mostly been studied with phenomenological models, which are calibrated for specific systems but cannot be easily generalized. Here, we propose a first-principle-based and thermodynamically-consistent micro-to-macro modeling approach for corrosion-induced cracking. Our model explicitly includes all relevant mechanisms, which are the release of ferrous ions at the steel-concrete interface, the diffusion of the products through the pores, the chemical reactions leading to the formation of rust (ferrous/ferric precipitates) [2], the stress build-up due to the pore-filling process, and finally the stress-induced damage of concrete when the material strength is exceeded. The pressure exerted on the pore walls due to a growing precipitate is quantified through the crystallization theory [3]. Our approach links the micro-mechanical processes (ionic diffusion, chemical reactions and stress development) with the macro-scale load-bearing capacity of the material and structure, and can be applied to any corrosion-susceptible system. Finally, we examine various properties of this complex heterogeneous system by analyzing the influence of the porous structure (porosity, pore size distribution) on the corrosion-induced cracking process and the overall material performance.

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Predicting Fracture Toughness ab-initio: Discrete Dislocation Plasticity Informed by Quantum-accurate Atomistic

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Predicting fracture toughness of bcc transition metals as a function of temperature is challenging since multiple mechanisms are activated, such as dislocation emission from crack-tip, debonding of crack-tip atoms, and interaction between crack and pre-existing dislocations. To capture the fundamental mechanisms that originate at the atomistic scale, extensive molecular dynamics (MD) modelling[1, 2] has attempted to reveal the crack propagation mechanisms which is important for predicting fracture toughness. However, no pre-existing dislocations are included in those atomistic models due to their expensive computational cost. This results in a predicted fracture toughness that is orders of magnitude lower than the experimental measurements[3]. A multi-scale approach is therefore required to enable the prediction of fracture toughness, whereby pre-existing dislocations are explicitly taken into account.

Here, to bridge the scales from the atomic to the micro-scale, we employ discrete dislocation plasticity (DDP), which is informed by a quantum-accurate atomistic model[3]. The atomistic model is validated on a broad range of properties that are crucial to simulate dislocation plasticity and fracture (elastic constants, surface energy, stacking fault energy etc.) The dislocation emission process from atomistic is analysed to obtain physical parameters as inputs for DDP. Based on the atomistic model, nudged elastic band calculations are performed to obtain the activation barrier for a number of dislocations, including screw, 71deg mixed, and edge type. A mixed mobility law is established subsequently. A cohesive zone model is used to describe the crack propagation. The dislocation emission process is incorporated by including Frank-Read sources near the tip. We implement corresponding changes in a 2D discrete dislocation framework [4].

To investigate the influence of pre-existing dislocations, we generate a series of initial dislocation distribution by loading and unloading of a rectangle specimen. The competition among crack propagation, dislocation emission from crack-tip, and thermally activated dislocation in the bulk is analysed. Next, the crack-blunting introduced by dislocation emission from crack-tip are studied by starting with different crack-tip geometry. The predicted fracture toughness is compared to experiments. Our work is a systematic approach to model fracture ab-initio up to the micro-scale, showing the necessity of a multi-scale approach for predicting fracture toughness.

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A Phase-Field-Based Chemo-Mechanical Model for Corrosion-Induced Cracking in Reinforced Concrete

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We propose a new model for the corrosion-induced cracking of reinforced concrete [1]. This complex chemo-mechanical phenomenon is of a great practical importance because it results in the spalling/delamination of concrete cover, and corrosion-induced damage is responsible for 70-90 % of prematurely deteriorated reinforced concrete structures.

The state-of-the-art knowledge of the underlying chemo-mechanical processes has been incorporated in three interconnected sub-models – (i) a reactive transport model for: (i.A) the transport of aggressive corrosion-activating species (such as chlorides) to the steel surface and (i.B) the transport and precipitation of iron ions released from the steel surface in the concrete porosity, (ii) model for the corrosion-induced pressure resulting from the concurrent constrained accumulation of: (ii.A) the rust layer in the vicinity of corroding steel rebar and (ii.B) the rust in the concrete pore space, (iii) a phase-field fracture model calibrated to accurately describe the quasi-brittle fracture of concrete. In addition, a damage-dependent diffusivity tensor has been employed to capture the enhanced transport of chlorides to the steel surface and the local reduction of the rate of accumulation of rust due to the enhanced transport of iron ions through cracks away from the steel surface.

The proposed model was numerically solved with the finite element method in COMSOL Multiphysics software. Several two-dimensional and three-dimensional numerical case studies were investigated including impressed current tests carried out experimentally in laboratory conditions. The comparison of experimental and numerical results revealed that the model can simultaneously capture the steel mass loss and the evolution of surface crack width for different concrete cover depths and applied corrosion currents. Also, for the samples with multiple rebars, the model accurately predicted the spalling or delamination patterns depending on the rebar spacing.

The results also indicated that corrosion-induced fracture could proceed with a partial saturation of the concrete pore space with rust. The rust was found to be largely in the vicinity of the rebar but also spread up to millimetres away from the steel surface, reducing the precipitation-induced pressure and delaying cracking. In regions with locally growing cracks, dissolved iron species were preferentially transported deeper into the cracks and precipitated there or in areas away from the steel rebar. Also, the enhanced transport of chlorides through cracks was found to importantly affect the resulting steel mass loss and the surface crack width. Parametric study revealed the profound influence of the porosity of concrete and the mechanical properties of rust, specifically Young's modulus and Poisson's ratio, on the resulting surface crack width, highlighting the need for appropriate characterisation studies of rust.

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Multiphysics modeling of electroactive polymer composites: A multiscale approach

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Electroactive polymers (EAPs) are a class of materials that demonstrate low-moduli, high strain capabilities, and ability to change their shape when stimulated by an electric field. Owing to their capability to undergo large deformation in response to the external stimuli, EAPs are considered 'smart materials'. In addition, EAPs have been nominated to be applicable in number of fields such as robotics, optics, acoustics and biomimetics. However, a high driving electric field is required for actuating the isotropic electric EAPs that may cause electro-mechanical instability and/or electric breakdown. This poor electro-mechanical coupling is attributed to the fact that the dielectric constant and flexibility in a polymer have an inverse relationship. Promising experimental works suggest that this limitation may be overcome by making electroactive polymer composites (EAPCs), which are flexible and have a high dielectric modulus [1].

With regards to the computational modeling of EAPs, a numerical scheme has been developed using a reduced mixed finite-element formulation for simulating the nonlinear response of isotropic EAPs. With regards to computational homogenization of coupled problems, an FE^2 framework was developed for the simulation of elastic dielectric materials at finite strains in [3]. The microscopic boundary value problem has been defined on periodic RVEs, and the developed method has been applied for the simulation of bimorph actuator made of EAPCs with ceramic inclusions. Furthermore, the two-scale scheme has been implemented for studying the behavior of heterogeneous magneto-rheological elastomers in the presence and absence of free space in [4], and it was demonstrated that the macroscopic response of a magneto-rheological elastomer strongly depends on the morphology of the underlying microstructure.

The aim of this research work is to provide an understanding of the mechanisms governing the electromechanical response of EAPCs undergoing large deformations. To this end, a multiphysics computational framework including the electro-mechanical couplings and the viscoelastic properties of the constituents will be presented. Generally speaking, phenomenological models provide a mathematical tool for material response, however, they are limited in modelling composite materials. Therefore, a computational homogenization that is based on the mixed finite element formulation at both the macro-scale and micro-scale (i.e. MFE^2) will be presented.

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Multiscale reduced order model for the analysis of damaging masonry domes and vaults

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The historical and architectural heritage of many European countries is composed of masonry structures, which suffered damaging processes due to their old building period and the peculiar mechanical properties of the material. Therefore, developing efficient numerical tools to evaluate their structural performance, especially under seismic loads, is a challenging task for the scientific community. Among the available methodologies [1], multiscale models, developed within suitable finite element codes, represent an effective procedure to describe onset and evolution of microcracks and follow the damage paths up to failure.

In this work, the multiscale formulation proposed in [2] is adopted to investigate response of masonry structures with periodic texture. Different structural models are assumed at the two scales of analysis, thus exploiting the advantages of each formulation. The constitutive response of the homogeneous Mindlin-Reissner shell considered a the macroscale is derived from the analysis of a representative three-dimensional masonry unit cell (UC). This contains all the geometric/constitutive information on the microstructure, being composed by elastic bricks bonded by potential damage/slip surfaces, modeled with interfaces elements. The homogenization process linking the two scales is based on the Transformation Field Analysis [3]. This procedure relies on the subdivision of the nonlinear regions of the UC, i.e. the interfaces representing mortar joints, in subdomains where prescribed variation of the inelastic quantities is assumed. The effect of macroscopic strains in the UC and that of the nonlinear quantities occurring in each subdomain is preliminary determined by performing a set of linear elastic analyses, which allow to determine proper operators to be used to solve the evolutive nonlinear problem of the UC within the multiscale simulation. Hence, the link of the two scales is obtained through a reduced order model that avoids the micromechanical modeling of the UC during the analysis, with indubitable computational advantages.

The model is implemented in a finite element code that uses a shear locking free thick shell formulation at the macroscale [4]. This is suitable for the analysis of both flat and curved masonry elements. Hence, the attention is here focalized on arches, domes and vaults, as these are structural elements largely adopted in monumental and urban buildings. Their overall behavior is studied in terms of load-displacement global curves and failure mechanisms. Damaging paths are in depth analyzed in view of a proper design of structural reinforcements aimed at improving the structural performance. The reliability of the results is proved by comparison with experimental data or solutions derived from detailed micromechanical simulations.

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Data-Driven Multi-Scale Analysis for Early Damage Assessment of Concrete Structures using Coda Waves

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The early detection and mitigation of damage in concrete structures can significantly decrease the cost of maintenance and repair associated with concrete infrastructure. Load-induced microcracking, a manifestation of weak material degradation, is a precursor to localized damage (macrocracking) in concrete structures and can be detected through the use of multiple-scattered late arriving ultrasonic signals, also referred to as coda waves [1].

In this study, a multi-scale approach combining computational modeling, wave propagation simulations, and machine learning techniques is employed to investigate the relationship between material degradation and coda wave variations at both the specimen and structural levels.

At specimen level, the virtual lab simulations of realistic mesoscale concrete models [2] are used to simulate damage initiation and progression at the specimen scale [3]. It is followed by wave propagation simulations on the virtual specimens at different levels of damage. Machine learning techniques are then employed to create a classifier for the prediction of damage based solely on the obtained synthetic ultrasonic coda signals [4, 5]. The classifier is validated using experimental coda signals obtained from laboratory tests.

At the structural level, the effect of boundary and geometrical conditions on coda signals is evaluated through 4-point bending simulations of a reinforced concrete beam. Finally, a strategy for predicting the state of damage at the structural level based on information from the specimen scale is presented.

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Bias-variance tradeoff in accelerating multiscale solid mechanics with Model Order Reduction and machine learning

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Recent advances in materials science and manufacturing techniques are enabling the advent of new high-performance material systems with highly-tailored microstructures. Together with a push for less reliance on costly and environmentally harmful experimental material characterization campaigns, these recent shifts underscore the importance of developing efficient high-fidelity multiscale analysis techniques. In particular, computational homogenization (FE^2) is seen as a powerful tool for unravelling small-scale phenomena in complex materials and linking them to macroscale performance with no loss of generality. Yet, FE^2 still does not see widespread application due to the extreme computational cost associated with embedding and solving microscopic boundary-value problems at each and every macroscopic material point. The development of effective ways to accelerate FE^2 simulations has therefore given rise to a new and highly-active research community.

A popular approach to accelerate computational homogenization is to substitute its costly micromodel computations by fast approximate solutions. Here, two main approaches can be distinguished: Model Order Reduction (MOR) techniques can be used to reduce the complexity of the original microscopic boundary-value problem based on snapshots of full-field microscopic solutions, or micromodels can be altogether bypassed in favor of machine learning-based surrogate models trained on homogenized stress-strain data. Although no consensus currently exists on a definitive approach with broad applicability, substantial progress in these two directions has been made over the last few years, in particular concerning accurate representations of highly-nonlinear and path-dependent microscopic material behavior.

In this work, we present an integrated overview of our recent developments in MOR- and machine learning-based tools for accelerating FE^2 simulations in solid mechanics. We frame and compare different methods not only in their ability to reproduce relevant material behavior but also in terms of their unique levels of balance between physics-based bias and data-driven variance. The discussion includes pre-trained and adaptive hyper-reduced projection MOR models for plasticity and fracture [1], active learning of constitutive models for composite materials with Gaussian Processes [2], hybrid data-driven surrogates with embedded physics-based constitutive models [3] and graph-based learning for full-field predictions of path-dependent microscopic behavior. We summarize our main findings along these fronts and provide a sketch of future research directions.

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Backward mode sensitivity analysis based multi-scale phase-field modeling

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In this contribution, we address the issue of generalization of formulation and efficient numerical treatment of multi-scale phase-field modeling of brittle fracture. The high numerical efficiency of the proposed formulation relies on backward mode sensitivity analysis. Sensitivity analysis has become an indispensable part of modern computational algorithms. Nowadays, the automation of sensitivity analysis enables efficient evaluation of sensitivities that are exact except for the round of errors. We propose a hybrid symbolic-automatic differentiation approach with code-to-code transformation and simultaneous stochastic expression optimization implemented in AceGen (www.fgg.uni-lj.si/symech/) as one of the most efficient approaches.

The automatic differentiation-based form (ADB form) of a classical phase-field formulation of brittle fracture [1] will be presented first. Next, the paper presents a unified approach to the development of an arbitrary mesh-in-element (MIEL) or FE^2 [2] computational scheme for two scale phase-field formulations. Implementation is based on efficient first-order (for FE^2 formulations) and second-order (for MIEL formulations) analytical sensitivity analysis, for which automatic-differentiation-based formulation [2] of essential boundary condition sensitivity analysis is derived. A generalized essential boundary condition sensitivity analysis-based implementation of FE^2 and MIEL multi-scale methods is derived as an alternative to standard implementations of multi-scale analysis, where the calculation of Schur complement of the microscopic tangent matrix is needed for bridging the scales. A fully consistently linearized two-level path-following algorithm is introduced as a solution algorithm for the strongly nonlinear multi-scale problems. Sensitivity analysis allows each macro step to be followed by an arbitrary number of micro sub-steps while retaining quadratic convergence of the overall solution algorithm [2]. The approach reduces the need for recalculation of global problems, consequently reducing the overall computational time. The approach also increases the concurrency of micro problems which can significantly improve the overall speed of the execution in multi-processor and multi-core systems. The paper also compares the benefits and drawbacks of the second-order forward and backward automatic differentiation approaches when applied to multi-scale phase-field modeling.

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Toughening effect analysis in problems of propagating cracks interacting with interfaces.

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Numerous fracture problems display, at the meso or microscale, phenomena involving the propagation of cracks interacting with interfaces. Examples where this mechanism plays a prominent role are: microcracks propagating in laminated composites, intergranular/transgranular fracture in polycrystalline metals, adhesive joints sandwiched between elastic substrates, crack bridging in structural ceramics, fracture mechanisms in biomimetics materials, among others. A notable result of such interactions refers to the possible effective structural toughening due to shielding effects induced by the interface on the propagating crack. Considering the high interest shown by this issue, the study of propagating cracks approaching interfaces has been the topic of intense research in the last few years.

In this work, following [1], we analyze the toughening mechanisms due to a propagating crack interacting with an interface at prescribed angles. The problem consists of a pre-cracked thin film bonded to a substrate, as adopted by [2]. The initial crack propagates toward the interface penetrating the substrate or deflecting toward the interface. In the last case, the film/substrate interface undergoes debonding. This effect inhibits the substrate crack penetration and may induce an effective structural toughness increase. Special attention is paid here to the unstable conditions arising from the shielding effect introduced by the interface.

The penetration/deflection mechanisms which are competing have usually been modeled using either stress-based criteria or energy-based criteria. However, it has been found that both criteria cooperate in the phenomenon. In the present analysis, we use a numerical methodology appealing to two different techniques. We compare the results obtained with: i) a phase field model characterizing the crack propagation across the film and substrate combined with a Cohesive Zone Model (CZM) characterizing the response of the interface (see [3]); and ii) a CZM for describing the crack propagation along the substrate and interface domains (see [4]).

The analysis is performed in the space of parameters defined by the ratio between the substrate and interface toughnesses, Γ_s/Γ_i, and the effective normalized load. The remaining parameters governing the problem, i.e. the characteristic lengths of the interface and phase field model, are also varied accordingly to assess their role in affecting the structural toughness increase.

Conclusions on the capacity of both numerical techniques to assess the apparent toughness and instability response are presented.

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Minisymposium NRFM:

Numerical aspects of regularized failure models

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

The time-step choice in regularized damage model simulations

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The choice of the time-step in regularized damage models as phase-field or Lip-field is seldom discussed. There is however a great interest in looking at this issue because it reveals difficulties in the simulation of regularized damage models.

In the presentation, we will consider three kind of models : a two-spring system, a 1D bar and, finally, several 2D geometries. For each model, we will consider both the quasi-static model (massless) and the dynamic model version. Regarding dynamics, explicit as well as implicit schemes will be considered.

The following topics will be discussed : time-continuity of the solution, snap-back, convexity with respect to the time-step choice, accuracy of the numerical solution with respect to analytical one (when available).

Having understood the impact of the time-step choice, we will then propose an automatic adaptive scheme for the time-step in order to reduce the computational time while keeping a given accuracy. The adaptive scheme allows to shift from explicit to implicit time integration and vice versa.

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Stabilized formulation for phase-field fracture in nearly incompressible hyperelasticity

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The phase-field fracture method has been well established within the context of linear elasticity. Ongoing work in soft materials extended the use of the phase-field model from linear to finite elasticity in a compressible setting where the Poisson's ratio, ν, ranged from 0.3 to 0.45. Staying within a compressible setting allows for pure displacement formulations to be used [1].

In this work we presents a stabilized formulation for phase-field fracture of hyperelastic materials near the limit of incompressibility. At this limit, traditional mixed displacement and pressure formulations must satisfy the inf-sup condition for solution stability. The mixed formulation coupled with the damage field can lead to an inhibition of crack opening as volumetric changes are severely penalized effectively creating a pressure-bubble. To overcome this bottleneck, we utilize a mixed formulation with a perturbed Lagrangian formulation which enforces the incompressibility constraint in the undamaged material and reduces the pressure effect in the damaged material [2]. A mesh-dependent stabilization technique [3] based on the residuals of the Euler-Lagrange equations multiplied with a differential operator acting on the weight space is utilized [4], allowing for linear interpolation of all field variables of the elastic subproblem.

This formulation was validated with three examples at finite deformations: a plane-stress pure-shear test, a two-dimensional geometry in plane-stress, and a three-dimensional notched sample. In the last example, we incorporate a hybrid formulation with an additive strain energy decomposition to account for different behaviors in tension and compression. The results show close agreement with analytical solutions for crack tip opening displacements and performs well at the limit of incompressibility. From an energy perspective the variational phase-field fracture model matches closely with theoretical critical initiation load (i.e., Griffith's criterion). The fact that the fully fractured configuration does not exhibit high residual pressures and stresses is a significant finding that has not been captured in prior results. This low-order formulation greatly increases computational efficiency for complex three-dimensional simulations, and has the potential to be extended towards dynamic fracture problems in soft materials at the limit of incompressibility.

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Adaptive mesh refinement and coarsening for the analysis of three-dimensional phase field fracture with discrete cracks

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Phase field models (PFMs) for material failure have been used to perform the fracture analysis of structures for crack initiation and propagation. In the PFMs, the total potential energy of a cracked elastic body can be given based on the variational approach combined with the Griffith's theory of fracture [1], wherein the variational principle to the potential energy leads to a minimization problem of the dissipation energy released to propagate a diffusive crack of damage phase field [2].

In order to accurately approximate the diffusive crack with high gradients of deformation and phase fields, the mesh in the damaged region should be sufficiently small compared to the characteristic length scale. Since a globally fine mesh for the analysis of phase field fracture demands on huge computational resources, an adaptive mesh refinement technique can be efficiently used to trace the crack trajectory with locally refine meshes. Although adaptive mesh refinement can improve the accuracy of solutions in the analysis of phase field fracture, very fine local meshes should be used near the crack tip and the crack surfaces. Accordingly, the computational cost significantly increases as the crack propagates because the number of elements along the crack trajectory increases rapidly.

A combined continuous-discontinuous approach can be used to enhance the efficiency of the analysis of phase field fracture by creating discontinuous discrete cracks for the fully damaged materials. Discrete cracks provide an accurate description of crack surfaces by detaching or eliminating fully damaged materials.

In this paper, we present a novel adaptive mesh refinement and coarsening technique using trimmed hexahedral (TH) elements for the analysis of phase field fracture with discrete cracks. An initial TH mesh is generated by cutting a hexahedral background grid with the boundary of a solid domain, as shown in Fig. 1. The boundary region is then composed of TH elements while hexahedral elements remain in the interior domain. Octree-based TH meshes are adaptively constructed from the initial TH mesh using an energy-based criterion during the analysis of phase field fracture, wherein the transition mesh interface is seamlessly connected by using compatible shape functions.

Discrete cracks are created by cutting octree-based TH meshes with critical damage isosurfaces that represent the crack surfaces. The crack surfaces of discontinuous discrete cracks can be then defined by the cut faces of TH elements. An energy-based criterion is employed to find the regions for mesh refinement. Mesh coarsening is also performed in the fully damaged regions with small amount of crack driving energy to reduce the computational cost. Fig. 2 schematically illustrates the octree-based mesh adaptation strategy for the analysis of three-dimensional phase field fracture with discrete cracks.

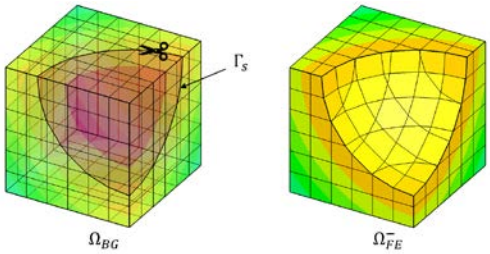

Fig. 1 An initial TH mesh generated by cutting a background hexahedral grid with the boundary of a solid domain.

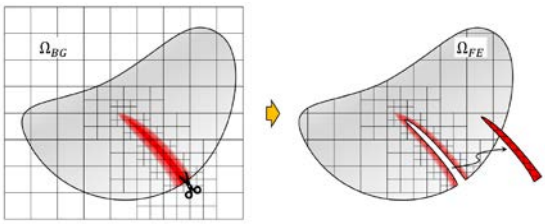

Fig. 2 Schematics of a discrete crack created by cutting an octree-based background mesh with critical damage isosurfaces for the analysis of phase field fracture.

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An adaptive phase-field method to model fracture propagation in orthotropic materials

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Several questions pertaining to the mechanical failure of composites remain unresolved despite significant advances in the composite mechanics. Many existing methods fail to accurately predict the various failure in composites, such as crack deflection, coalescence, and matrix cracking at the laminate interfaces. We extend a recently developed adaptive phase-field method, initially proposed for isotropic material [1], to model delamination in the orthotropic laminated composites. A penalized second-order structural tensor is introduced in the crack-surface density function to facilitate preferential crack growth in the direction of fiber orientation [2]. Furthermore, crack driving force was divided into individual fiber and matrix damage corresponding to different failure modes in the laminate [3]. The primary motivation is to predict the damage regions and complex crack patterns in laminate under various loading conditions by formulating a robust numerical model. This will lead to study different failure mechanisms (translaminar, interlaminar and intralaminar) that prevails in laminate.

In this work, we integrated orthotropic phase-field model with adaptive refinement technique strategy to accurately predict crack propagation in orthotropic materials. The continuity is enforced in weak form through Nitsche's method at the interface of refined and standard elements. The developed approach is then validated through several benchmark numerical experiments revealing the complex fracture mechanics inside composite. The results demonstrate that the crack has an affinity to propagate in the direction of fiber orientation, which is also validated against experimental results. Furthermore, parametric studies are performed to evaluate the damage evolution and maximum load-carrying capacity of the laminate considering interphase material between alternate lamina by varying one property at a time.

It is computationally expensive to perform three dimensional (3D) analysis of composite. A 3D visualization of failure in composite laminate is studied then by conducting two dimensional (2D) analysis of 3D laminate incorporating different orthographic projections (front, side, and top views of laminate). The existing model will study the damage evolution in laminate from meso-scale to macro-scale.

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Extension of phase field method for predicting fracture path in bi-materials by strong-form meshless method

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Material failure prediction is an essential engineering practice for the life-cycle prediction of components. Present computational fracture mechanics uses, either a discrete or diffused, crack model to predict the fracture path. Traditional discrete methods require an additional ad-hoc criterion for the crack path propagation, making it more computationally intensive for complicated scenarios like crack-branching, crack interaction, crack-path propagation across an interface in composite materials and for three dimensional geometries. On the contrary, continuous approaches like phase-field make these predictions smoother as they use a continuous displacement field with an intrinsic length scale thus controlling the width of transition zone. In the case of phase-field based model, the crack is represented by a scalar field, and the evolution of phase-field evolution equation leads to the modelling of crack path [1, 2].

The present work deals with developing a numerical model for capturing the fracture propagation by phase-field technique in a bi-material (isotropic and specially orthotropic cases). The phase field damage model will be implemented, employing the strong-form meshless local differential quadrature method [3], coupling with the mechanical equilibrium equations.

Strong-form meshless methods can solve governing equations employing lesser discretised nodes without compromising on the accuracy thus making them an ideal candidate for multi-physics problems [3, 4]. The present work implements a strong-form technique called the local differential quadrature (LDQ) method [5]. The LDQ method is capable of solving strong-form governing equations employing uniform, cosine, or random nodes. Despite the advantages offered by LDQ method, solving boundary value problems for bi-material involves an unique challenge of ensuring the traction continuity across the bi-material interface (unlike in finite element method), which is addressed in the present work.

The *novelty* of present work is to demonstrate the numerical implementation results of phase field method with mechanical equilibrium equations, for *bi-material* case, employing LDQ method ensuring a correct traction continuity (currently lacking in the literature).

The present phase-field model will be based on Miehe *et al.* [2] involving a history variable (irreversible damage) and solving the problem using a staggered approach. The capability and the correctness of the formulation will be tested using different benchmark problems, wherein the effect of individual layer material stiffness on the propagation of fracture path is observed.

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Numerical modelling of three-dimensional fracture propagation in layered materials using parallel computing

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Detection and tracking of cracks are of significant importance in engineering analysis and design. This is due to the high maintenance and repair cost of the damaged structures. Cracks initiating from the surface of the material may penetrate into the interior when subjected to loads. Furthermore, the spatial pattern of these cracks could be very complicated and may not be easily predicted using traditional theoretical and experimental methods. As such, there is a need to develop robust numerical models that help in the analysis of crack growth so as to develop efficient strategies to combat the issues arising from the growth of inherent defects and cracks [1].

Recently, phase-field method has gained in popularity for modelling crack propagation [2]. In the phase-field method, fracture is treated as a smeared zone in the continuum that has completely lost its mechanical strength. These models offer several advantages. Firstly, they offer a means to model arbitrary crack paths independently of the underlying finite element mesh. Secondly, they adopt an energetic approach to dictate both the initiation and propagation of damage. Coalescence and branching are naturally treated within the framework as damage is obtained as an additional nodal field on a given background mesh [3].

However, a major weakness of the phase-field method is its high computational cost. This method achieves mesh objectivity by regularizing the crack over a band of finite elements with some minimum bandwidth. As such, a two-dimensional domain requires meshes in the order of 10^6 elements and a three-dimensional domain requires meshes in the order of 10^9 elements. This colossal computational cost prevents the method from being utilized in realistic engineering applications at present.

In this study, we develop a robust three-dimensional phase-field model to simulate crack propagation in layered subsurface systems, by leveraging parallel computing. We implement the hybrid phase-field model of Ambati et al. [3] in deal.II–an open source finite element library [4]. This model will then be utilized to perform several numerical experiments and examine the effects of contrast in parameters such as elastic stiffness, fracture toughness and interface inclination on fracture propagation in layered subsurface formations with perfectly bonded interfaces. Conclusions will be drawn on the conditions that result in fracture arrest, deflection and penetration at layer interfaces in layered formations.

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Investigating Brittle Fracture with an Adaptive Phase-Field Model using the Scaled Boundary Finite Element Method in Three Dimensions

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The phase-field method (PFM) has been successfully applied to simulate damage mechanisms in a wide range of materials including ceramics, metals, and polymers. It has also been used to study various types of loading such as tension, compression, and shear. The PFM has proven to be a powerful tool for understanding and predicting the behavior of crack propagation in materials. This method represents the crack by regularizing its surface over a small width, referred to as the length scale. To simulate the steep variation of the phase-field, a very fine mesh is needed in the damaged area, which leads to high computational costs, particularly if a uniform mesh is used [1]. However, the use of adaptive mesh refinement techniques can help to reduce the computational cost and increase the accuracy of the simulations.

In this research, we develop an adaptive phase-field simulation of fracture in 3D by utilizing an automatically generated octree mesh, analyzed through the scaled boundary finite element method (SBFEM). The simulations rely on 3D digital images as inputs. The mesh is automatically generated from these digital images, where the size ratio between two adjacent hexahedrons is limited to 2:1. This mesh configuration ensures a limited number of unique elements according to the position of the hanging nodes and thus contributes to reducing the computational effort and resources.

The analysis of the automatically generated octree mesh is performed using the scaled boundary finite element method (SBFEM). This semi-analytical method simplifies the analysis of polyhedral elements. Here, only the discretization of the faces of the domain is required [2]. Adaptive mesh refinement is achieved using an error indicator based on the SBFEM solution. This allows for a more efficient use of computational resources by only refining the mesh in areas where it is necessary. The staggered solution scheme outlined by Miehe et al. [2] is used to solve the system of coupled nonlinear differential equations for the phase-field variable and the displacement. The hybrid phase-field method is adopted, assuming that the phase-field evolution is driven only by the elastic tensile energy, resulting in linear differential equations for the displacements [3]. To evaluate the performance of the proposed method, several 3D benchmark examples are presented. These examples demonstrate the accuracy and efficiency of the proposed method and its ability to handle various types of fracture problems.

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Robust solvers for "Lip-field" damage models

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Models formulated within the framework of the Continuum Damage Mechanics are often used to simulate cracking in quasi-brittle materials. However, when the material softens, the solution to the equilibrium problem is no longer unique. In the context of the finite element method, this leads to a pathological dependence on the finite element mesh used to discretize the computational domain.

Moës and Chevaugeon [1, 2] recently proposed a new way to avoid spurious localizations. The idea is to impose a Lipschitz regularity on the internal variables controlling material softening. Such a regularity constraint introduces a characteristic length into the formulation. The solution to the problem is sought by alternated minimization of a convex incremental energy potential with respect to the unknown displacement and damage fields. The convex Lip-field condition is added as an additional constraint in the alternating minimization. Upper and lower bounds built from a prediction of the local evolution of the field of damage make it possible to optimize the search for the regularized damage field.

The first aspect treated in this contribution concerns the formulation of the minimization problem to be solved for computing the regularized damage field. It is shown that if the desired solution is obtained by combining the upper and lower bounds, the minimization problem can be rewritten differently, and the resulting numerical formulation gains in stability while keeping a final solution respecting the Lipschitz constraint. Calculation times are also reduced.

The second aspect concerns the formulation of path-following solvers dedicated to the "Lip-field" approach to damage. Adapting the external loading during the calculation (see e.g., [3, 4, 5]) to control the evolution of the material non-linearities is helpful to obtain a solution even in the presence of structural instabilities and to reduce the number of iterations to convergence. This second aspect is of paramount importance. Indeed, using indirect loading control algorithms (if well chosen and formulated) can significantly reduce the number of iterations to converge in the context of an alternated minimization solver.

After illustrating the numerical formulations, some one-dimensional and two-dimensional test cases are presented.

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Dual-mesh approach to discretisation for phase-field fracture method

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The Phase-field (PF) method for fracture problems was the subject of extensive research during the last decade. Its popularity can be attributed to two advantageous properties that arise from the diffusive crack description and variational approach to fracture, namely simplicity and versatility.

However, some specific disadvantages are inherited from the method's regularized formulation that contains a length-scale parameter. Besides governing the PF diffusivity, often the length-scale is considered as a material parameter, coupled with the material's critical stress, leading to the fact that the length-scale cannot be chosen arbitrarily. As a smaller length-scale leads to sharper gradients of PF and material stiffness, mesh density requirements are also determined by the length-scale. Hence, the disadvantage comes from the fact that simulations with a small length-scale require very dense meshes, and therefore lead to large computational costs.

Several works addressed the problem of computational costs due to mesh requirements. The most obvious approach is managing a number of degrees of freedom by means of adaptive remeshing. So far, the most promising adaptive approaches are anisotropic ones [1]. Further, computational costs can be reduced by utilizing phase-filed methods that exhibit better convergence, like the fourth-order methods [2] that have a smooth PF profile at the peak, but unfortunately require discretization with the C^1 continuity of PF. Lastly, the utilization of special discretization techniques can be utilized. Herein, the work of Olesch [3] can be noted, where exponential shape functions were utilized for a better approximation of PF profile. On the other hand, Sargado [4] hypothesized that mesh sensitivity within the Finite Element Method (FEM) framework comes from the fact that FEM is not optimal since the PF profile contains a cusp. To resolve such a problem, a combined discretization with FEM for displacements and the Finite Volume (FV) method for PF was proposed, where PF data were stored in the center of the element/volume. The resulting method reduced spurious fracture energy and showed better convergence in comparison to the standard FEM approach.

This contribution follows the ideas of Sargado [4], but instead of using FV, the new approach is based on the construction of a new (secondary) mesh from nodes positioned at the element centers of mesh used for displacements (primary mesh). The new mesh contains linear polygonal finite elements or linear triangular elements obtained by triangulation of polygons. The benefit over the FEM-FV approach is that the local part of fracture energy is not constant over the primary element, i.e., does not contain PF plateaus, and hence the local part of critical energy is not overestimated as in the FEM-FV approach. Results of benchmark examples show that the proposed method clearly leads to better convergence of critical force for problems with a sudden crack propagation, while for a stable crack propagation, results can be considered only marginally.

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An enriched phase-field approach for the efficient simulation of fracture processes in 2D

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During the last decade, the phase-field method for fracture has become one of the most popular approaches for the simulation of cracks and their propagation. The main advantages of the phase-field method are its easy implementation and its capability to automatically detect when, in what direction and how far a crack propagates without the necessity for additional criteria. Even crack branching and crack coalescence are captured automatically. The phase-field method has been applied to brittle and ductile fracture and to quasi-static and dynamic crack propagation. Inherent to the phase-field theory of fracture is a small length scale parameter which is responsible for the width of the smeared crack reflected by the phase-field. In the classical phase-field method, the element size needs to be significantly smaller than that length scale parameter leading to very large meshes even for 2D problems. In addition to that, even for linear elastic fracture mechanics problems, a phase-field formulation leads to a highly nonlinear finite element problem. The combination of very fine meshes and high nonlinearity leads to an enormous computational effort which is the biggest disadvantage of the phase-field method.

In contrast to the phase-field method, the extended finite element method (XFEM) or the generalised finite element method (GFEM) are able to capture the discontinuity of the displacement field due to a present crack within an element very accurately by means of properly defined enrichment functions. These enrichment functions require a geometric description of the crack position e.g. by means of an additional explicitly given mesh for the crack surface or by means of level sets. For the XFEM/GFEM it is also necessary to evaluate additional criteria for crack propagation simulations. The biggest advantage of the XFEM/GFEM is its rather low computational effort even for 3D simulations and the mesh independence of the sharp crack geometry. However, due to the necessity for an additinal geometric representation of the crack and the dependence of the enrichment functions on the crack geometry, the simulation of e.g. crack coalescence or crack branching in 3D is rather difficult.

In the present approach we combine the advantages of the phase-field method with the advantages of the XFEM/GFEM. The extended phase-field method (XPFM) [1] is based on a classical phase-field approach for which a locally transformed ansatz is chosen for the phase-field and an enriched ansatz similar to the XFEM/GFEM is chosen for the displacement field. The enrichment function for the displacement field is based on the phase-field. As a consequence, an additional geometric representation of the crack is not necessary to evaluate the enrichment function. The transformed phase-field ansatz in addition to the enriched displacement field ansatz allow for significantly coarser meshes compared to the classical phase-field method as well as displacement discontinuities within elements similar to the XFEM/GFEM. Various examples in 2D compare the performance and accuracy of the XPFM approach with the classical phase-field method.

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Minisymposium QBC:

Quasi-brittle cracking, coupled processes and hydraulic fractures

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

Leapfrog in Computational Fracture Mechanics Enabled by Curvature-Limiting Sprain as Localization Limiter and Inspired by Gap Test

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Sixty-one years after Ray Clough's epoch-making finite element analysis of cracks in Norfolk Dam [1], there is still no completely satisfactory computational model for fracture. This is evidenced by recent model comparisons with many *distinctive* [2] fracture tests—tests to be distinguished from the *nondistinctive* ones, i.e., those that can be fitted closely by very different models. The distinctive comparisons reveal dismal performance of peridynamics and severe applicability limitations of the phase-field models [3,4], as well as certain innate inadequacies of the nonlocal models of integral and gradient types. The crack band model (CBM) [5] with microplane model M7 is found to give relatively much closer fits of the test data, especially the gap test [6,7] and size effect [5], mainly thanks to its realistic crack-face boundary conditions. Yet the CBM has three limitations: 1) the width of the band front cannot be varied, 2) the damage distribution across the band cannot be resolved, and 3) regular meshes cause bias of the propagation direction. All three are overcome by the new smooth CBM (sCBM) [6]. Its idea is to limit damage localization within a band of multi-element width, equal to the material characteristic length, by restricting the displacement curvature through sprain energy density Φ, which represents energy homogenization, distinct from the standard stiffness-based homogenization. Called the sprain energy, Φ is not the strain energy. Rather, it is the Helmholtz free energy density of the third-order tensor of the curvature (or second gradient) of the displacement vector field, briefly called the sprain (a term inspired by ligament sprain in medicine). The sprain includes material rotation gradient is not expressible in terms of the strain-gradient tensor. The derivatives of Φ with respect to finite element nodal displacements yield self-equilibrated sets of in-plane nodal of body (sprain) forces resisting excessive softening damage localization. In the simplest version [8] using constant-strain finite elements, some sprain forces were applied as nodal forces of distributed body forces of adjacent elements. The ways of overcoming this programming inconvenience are outlined. The sprain forces act only during softening damage. Numerical results confirm good performance and close fits of distinctive concrete fracture tests.

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Objective numerical evaluation of cracking in quasi-brittle materials via adaptive mesh and formulation refinement

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The numerical analysis of localized structural failure using the standard displacement-based finite element (FE) formulation from solid mechanics has shown to produce results spuriously dependent on the mesh employed to perform the calculation. Crack trajectories and failure mechanisms computed with this approach present the critical issue of being spuriously dependent on the orientation of the FE mesh used to evaluate the problem.

In the past, this aspect has been resolved by the authors via the employment of a mixed strain/displacement finite element formulation to perform the nonlinear solid mechanics analysis. This method guarantees the local convergence of the problem, allowing to produce mesh bias objective calculations [1-2].

For the efficient analysis of quasi-brittle fracture, the present work proposes adoption of an Adaptive Formulation Refinement (AFR) scheme [3]. This approach allows to start the simulation using the standard displacement-based FE formulation, and to adaptively activate the mixed FE method only in the areas where the crack develops while the standard formulation is maintained in the rest of the structure. This enables to introduce very significant savings in computational cost while maintaining the accuracy and mesh objectivity in the calculation of the crack path provided by the mixed FE.

The AFR method is combined with the adoption of an Adaptive Mesh Refinement (AMR) strategy to further increase the efficiency of the computations [3]. With the proposed octree-based AMR scheme it is possible to adaptively refine the mesh only in certain areas of the domain. This allows to initiate the analysis with an initially relatively coarse mesh and to introduce its refinement only where the cracks develop. With this strategy it is possible to reproduce the phenomenon of cracking with the sufficient accuracy while preserving a reasonable computational cost of the simulation.

The nonlinear behavior of the material is reproduced through the adoption of local isotropic and orthotropic damage models. Within the proposed framework, the local format of the problem of fracture is preserved, without inserting regularizing terms in the variational form. Neither are gradient or higher order terms introduced in the constitutive law.

The accuracy and cost efficiency of the proposed framework is examined through an extensive set of numerical simulations of benchmark problems as well as experiments. Computations show that the combination of the AFR and AMR strategies allows to produce mesh objective results in terms of crack trajectories, collapse mechanisms, load capacity and nonlinear response. Experimental results are reproduced with precision in 2D and 3D.

The comparative assessment of the proposed AFR scheme with corresponding computations using the standard FE formulation only is performed, showing the superior performance of the AFR approach in terms of result quality. Computational efficiency of the methodology is examined as well, showing its ability to produce very significant savings in computational cost while allowing to provide mesh bias objective results.

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Some comments on modelling failure with peridynamics

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Peridynamics have been widely developed over the past twenty years following the pioneering work of Silling (2000). Because conservation equations do not involve the derivatives of the displacements (i.e. strains), it is a convenient framework for modelling fracture. The theory captures very easily the initiation and propagation of discontinuities of displacements in a structure. This convenient property, however, is counterbalanced by the difficulties at handling Dirichlet or Neuman boundary conditions. This aspect of peridynamics is well known and it has been discussed in detail.

Peridynamics is a nonlocal theory that accounts for long range interactions, as inspired by molecular simulations. The mechanical response at each material point results from an average of interaction forces taken over a domain called "horizon". So far, the horizon has been considered to be a numerical parameter. This paper intends to demonstrate that it should not be the case. In the present contribution, we shall consider bond-based interactions only.

We illustrate the argument on a simple, one-dimensional, problem of propagation of waves and their interaction. We look at the failure of the bar triggered by the interaction between two constant strain waves at the center of the bar. When the waves meet, the strain is multiplied by two and failure is initiated. Two interaction models are considered. An elastic perfectly brittle interaction and a damage model with linear softening after the peak force has been reached. In the first model, the parameters are the micro-stiffness and the critical stretch, the softening slope is added in the second.

The profiles of strain and damage upon fracture are obtained. The width of the strain profile is found to increase linearly with the horizon size, similar to what is observed in continuum based nonlocal models for fracture. The horizon has the same role as the internal length and therefore should bear the same status. According to a continuum model, material parameters are the elastic constant, the tensile strength, and the fracture energy. Usually, in peridynamics, the horizon is defined arbitrarily and the peridynamics parameters are adjusted to fit these parameters. We show that such a fit is not possible unless the horizon becomes a material parameter, useful for the calibration of the fracture energy. Without this, the tensile strength corresponding to the correct fracture energy for a given horizon size becomes unrealistic.

Consequence of the crack tip microcracking statistics on dynamic nominally brittle fracture at the continuum-level

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Linear elastic fracture mechanics correctly models dynamic fracture as long as its application assumptions are verified and a single crack is considered [1, 2]. Locally, the elastic energy release rate must be equal to a material constant, the fracture energy. In contrast, in nominally brittle materials undergoing rapid fracture, the collective dynamics of nucleation, growth and coalescence of numerous microcracks in the near-end region implies a strong dependence of fracture energy on cracking rate, the modelling of which remains a theoretical challenge [3, 4]. Here, microscopic statistics from experimental reconstructions of microcrack dynamics are compared to a refined geometric model.

The experiment were performed on Polymethylmethalcrylate (PMMA), fracture speed, v and stress intensity factor K were determined by potential drop method and finite element analysis. The microcracking processes in the process zone occurs at nanosecond/micrometer scale, *a priori* beyond the reach of standard experimental mechanics methods. However, the microcracks that form near crack tip at high enough fracture speed (for $v > v_{mc} \simeq 0.2c_R$ [5]) have the particularity to leave characteristic conics patterns onto the fracture surfaces [3] which can be analysed post mortem and allow a complete recondstruction of the dynamic [4].

The probability distributions that control the jumps in time and space between microcracks are determined experimentally. Nevertheless all these treatments are very difficult and the range of available parameter is experimentally limited. To overcome this problem, we develop a dynamic random sets model to artificially generate all the damage dynamic. We first check that the model is indeed able to reproduce all the experimental data. Then we extend it to a larger range of parameters and we extract scaling laws between the statistics at the microscopic scale and a control parameter that we choose equal to $d_n \sqrt{\rho}$.

The comparison to experimental data shows that finally these dynamics are entirely determined by two constant, the constant propagation velocity of microcracks and a length scale related to their share in the fracture energy. The areal density of the nucleation centres of the microcracks then controls the dynamic. The upscaling of this geometric microcracking model provides a robust crack growth law at a continuous scale. The three parameters of this model can be fitted to both microscopic and macroscopic data. A clear interpretation of the variation of fracture energy with fracture rate is obtained.

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Mixed-Mode Fracture of Cement Paste and Interface under Three-Point Bending Test: Numerical and Experimental Investigations

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Concrete is a quasi-brittle material with a high degree of heterogeneity. The presence of multiple phases in concrete (cement paste, sand, gravel, porosity, etc.) leads in a gradient of mechanical characteristics, notably around the aggregates, where an Interfacial Transition Zone (ITZ) is formed. This disparity in microstructure characteristics has a significant impact on the process of damage and cracking, making fracture propagation in concrete difficult to predict.

The cracks can occur at the interfaces of relatively heterogeneous materials like concrete due to debonding and subsequently spread through the cement paste, or vice versa [1]. These observations highlight the significance of conducting a local numerical investigation of crack propagation at the level of pure cement paste and at the interface between the cement paste and the aggregate, considering these two areas to be preliminary cracking zones. The CZM is one of the modeling methodologies used here for fracture mechanisms in heterogeneous materials [2]. This model allows us to define the fracture as a displacement jump between cohesive elements. The CZM model will be used to execute a numerical study of mixed mode fracture at the "local scale" of cementitious material [3,4].

For this purpose, two-dimensional simulations of three-point bending tests under variable load and geometry are modeled by employing CZMs. These tests are performed on parallelepipedal samples of dimension (10 x 10 x 30 mm^3).

A pre-notched cement pastes samples beam with eccentric load are tested. The eccentricity is defined as the distance between the point of load and the center of the sample. Four loading points equal to 0 mm (centered load), 2.5, 5, and 7.5 mm are studied. Composite specimens (cement paste linked to one siliceous aggregate) are also evaluated in bending with centered loading. Here, the composite specimen design is different: the interface angle between cement paste and aggregate varies between 30° and 90°.

This procedure enables the provision of a diverse set of crack trajectories and propagation modes, enhancing the calibration of numerical models by comparison with experimental results at this local scale.

As result, the numerical responses match the experimental results after identifications of the elastic and cohesive parameters based on experimental data. Therefore, the findings at this local scale demonstrate that when the mixed mode ratio increase, the fracture energy and material resistance increase too for the two sample types (cement paste and composite). Moreover, similar crack propagation, fracture path and mechanical responses are obtained in experimental and numerical model.

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Modelling Freeze-Thaw Behavior of Cementitious Materials

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Frost damage is one of the most important factors affecting the durability of cementitious materials in regions with cold climates. Over the years, many theories have been proposed to explain this complex phenomenon. Frost induced damage can be categorized as internal cracking and surface scaling. Damage due to internal cracking leads to lower material stiffness modulus, drop in tensile strength and increase in porosity and permeability. Surface scaling, which is most commonly associated with the presence of solutes, results in material surface loss at a solute concentration of roughly 3%.

The freezing behavior of cement-based materials under fully saturated condition has been experimentally investigated by a number of researchers. Experimental test results reported by Zeng et al. [1] showed that the ice saturation degree is influenced by both porosity and pore connectivity. Additionally, the test findings by Zeng et al. [1] demonstrate that as the number of freeze-thaw cycles increases, concrete's compressive strength, flexural strength and splitting tensile strength decrease.

Several models have been developed over the years to predict the thermo-mechanical behavior of porous building materials such as cement paste subjected to frost action. Powers introduced the famous hydraulic pressure and osmotic pressure theories, which constructed the basic theory of frost damage [2]. A mathematical model based on the pore size distribution and desorption and absorption isotherms for concrete below and above 0°C was established by Bažant et al. [3]. Despite the proposed models by several researchers, freezing process in porous media, such as concrete, still remains a very complex topic. The process involves interaction between heat transfer and moisture, phase change and deformation.

The main goal of the present study is to numerically investigate the freeze-thaw behavior of two different cement pastes saturated with variable chloride concentrations. With this purpose, the 3D coupled hygro-thermo-mechanical (HTM) model [4], implemented in the in-house FE code MASA [5] is employed. The mechanical part of the model is based on the microplane theory [6]. The coupling between the mechanical (loading) and non-mechanical processes (freeze-thaw processes) is ensured by using the staggered solution procedure.

The model is first validated using a numerical and experimental study available in the literature [1]. It is shown that the model can well capture the freeze deformation during the initial cooling phase. Moreover, as a function of porosity and pore size distribution, the same as the experimental tests, the numerical results show initial contraction followed by expansion when the temperature drops below the freezing point of the pore solution. The validated model is then used to study the effect of the liquid water permeability and elastic modulus of the hardened cement paste on the freeze-thaw behavior of the material.

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Cracking and Fracture of 2D and 3D concrete specimens subject to External Sulfate Attack

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Amidst the numerous ways in which concrete can undergo degradation, this research aims to examine the phenomenon of external sulfate attack as a type of chemical degradation.

Concrete, being a heterogeneous material, can display different internal structures and constitutive behaviors depending on the level of observation used in the investigation. The meso-level is an intermediate level of analysis in which concrete is considered to consist of a homogeneous mortar matrix surrounded by coarse aggregates. In the context of finite element analysis, the weakest part of the meso-structure and the areas of possible fracture are represented here using zero-thickness interface elements, sometimes also called cohesive elements. These elements are placed in the regions where the aggregates meet the matrix and within the matrix itself, highlighting the zones where concrete is most vulnerable.

From a mechanical perspective, non-linear behavior is assumed to take place solely at the interface elements. In order to model this behavior, a constitutive law that combines both elasto-plasticity and fracture mechanics is utilized for these elements. On the other hand, for the rest of the concrete structure, a linear elastic constitutive model is employed [1].

With regard to the reactive transport problem, the model is based on the pioneering work of Tixier and Mobasher [2]. This work was first introduced in a meso-mechanical analysis with interfaces by Idiart et al. [3] in two dimensions and later expanded incipiently to three dimensions by Pérez et al. [4].

The coupled analysis was performed using a staggered method in which the two problems were cyclically solved. The reactive transport results were first obtained and then used as input for the subsequent solution of the mechanical problem. This cyclic approach allowed for a more accurate and comprehensive analysis, as the results of each problem influenced the solution of the other. The problem is addressed by utilizing the DRAC5 program, which was developed by the MECMAT research group at the Universitat Politècnica de Catalunya (UPC). In recent times, the parallelization of the code has significantly enhanced its capabilities, enabling the analysis of progressively larger meshes.

In this paper, the numerical model is described and the results obtained from both 2D and 3D cases are analyzed and discussed. Special attention is paid to the capability of the approach to reproduce the experimentally observed cracking patterns, such as the “onion peeling” effect, as well as the numerical performance of the parallel implementation including scalability with no. of processors.

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Coupled DDM-FEM solution applied to fault reactivation assessment in CO_2 sequestration

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The amount of CO_2 in the environment has increased due to widespread industrial activities, fossil fuel utilization, as well as deforestation. Carbon sequestration and geological storage are the most used and promising techniques to mitigate carbon emissions [1]. Alternatively, carbon storage can also be utilized for enhanced oil recovery, improving reservoir permeability and reducing CO_2 emissions from petroleum activities. However, the capture capacity and long-term safety in geological deposits must be ensured since CO_2 leakage through geological faults can potentially contaminate the soil and groundwater surrounding the storage site.

This work proposes using a Displacement Discontinuity Method (DDM) and Finite Element Method (FEM) coupling scheme to investigate fault reactivation due to Co2 injection in a pre-salt reservoir. The coupling approach adopts the finite element methods to solve the fluid flow through the porous media associated with the Displacement discontinuity method to solve the mechanical behavior [2]. The geological faults are modeled using a zero-thickness interface element associated with the Mohr-Coulomb plastification criterion to evaluate the fault reactivation process [3].

The influence of the in-situ stress and the fault orientation on the reactivation potential are analyzed. The simulation also investigates the optimum injection pressure to maximize CO_2 storage and critical reservoir pressure to avoid fault reactivation. The simulation indicates that reactivation can increase the storage capacity, in other cases, it can result in corridors for leakage of injected CO_2. Furthermore, the depleted petroleum reservoir overlayed with salt caprock could be suitable for long-term and safe carbon capture and storage in geological formations.

The numerical results show that the coupled DDM-FEM approach can be an attractive alternative to simulate fault reactivation in CO_2 storage process with good accuracy and low computational effort.

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A fully coupled finite element model for simulating hydro-dynamical plugging of unwanted hydraulic fractures in wellbore strenghtening

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For a successful drilling operation, a proper mud weight must be maintained between two limits. The pore pressure gradient being the lower and the fracture pressure gradient of the formation being the higher one. These limits are often called the "*mud weight window*". It is possible that this range may become too narrow under certain conditions like drilling in deep or ultra-deep-water, construction of highly deviated wells, passing through depleted zones and penetrating naturally fractured zones. In such cases an unwanted hydraulic fracture may be induced thereby causing the loss of drilling fluids in the surrounding formations with an estimated annual loss to the global drilling industry of about 2-4 billion [1-5].

Wellbore strengthening, often shortened to WBS, usually incorporates the addition of lost-circulation materials (LCMs) of various sizes, types, and mechanical properties to the drilling fluid. These particles are intended to plug the induced or natural fractures that cause damage to the wellbore. This way, the maximum pressure a wellbore can tolerate is increased artificially so that mud losses are diminished. Hence WBS intends to enhance the effective fracture pressure and widen the mud weight window rather than actually increasing the strength of the formation. In particular, these techniques aim to alter the stress distribution near the wellbore and the fluid pressure inside the fracture to increase the maximum sustainable pressure of a wellbore without propping unwanted hydraulic fractures. The efficiency in arresting the unwanted induced hydraulic fractures works by bridging, plugging, or sealing the unwanted hydraulic fracture [1-3]. The physical mechanisms through which LCM operate are not fully understood. Current hypotheses regarding these mechanisms are: the stress cage [6,7], fracture closure stress [8,9], and fracture propagation resistance [10,11].

An open question that exists is the efficiency of the plug and its implications on the stress change during plugging. In the impermeable formation, a plug may be perfect if it completely isolates the fluid from reaching the tip or it may allow some fluids to reach the tip. If the fracture is plugged in a permeable poroelastic formation, the plug cannot be perfect as the pressure behind the tip balances the pressure of the formation and that of the invasive fluids. Thus, the influence of bridging on the closure stresses provides useful information about the effectiveness of plugging.

In this work, we investigate with the finite element method the fully coupled stress change in impermeable and permeable strong formations, by creating and allowing an unwanted hydraulic fracture to propagate up to 5m (in the toughness dominated regime) and then plugging it, to obtain numerically the in-situ stress change at the location of the tip and the plug. The toughness dominated regime implies that most of the energy in the process is expended in fracturing the rock rather in the viscous fluid flow which is more suitable for short fractures. Furthermore, the toughness dominated regime finds applications in ultra-deep formations where the fracture propagates in a highly compressive stress state and most of the energy is expended in splitting the rock. After plugging the fracture, the in-situ stresses are recovered and a critical evaluation of the stress change is performed to assess the effects of the efficiency of the plug on the closure stresses [14,15].

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Fluid flow and fracturing in weakly cemented porous media: an insight into the underlying mechanisms

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Fluid flow and fracturing in porous media are the underlying mechanisms of many applications in the fields of energy geomechanics, hydrogeology and groundwater hydrology. The characteristics of the fluid flow vary depending on the physical and mechanical properties of the porous medium and the composition and viscosity of the injected fluid. These parameters are chosen depending on the target of each application (whether fracture or uniform replacement of pore fluids - infiltration) and the depth of the operation (soil/rock) [1].

Many operations take place in weakly-cemented and poorly-consolidated sands which represent the host rock for a large portion of active aquifers and oil and gas reservoirs. These materials have much higher porosity and permeability compared to strong rocks, hence, their behaviour under fluid injection conditions is very different and largely unexplored [2].

Since coring of such formations is problematic due to large costs and destruction of cementation, synthetic materials of known mechanical and hydraulic properties were generated to perform fluid flow injection experiments [1], [3]. The method used to prepare the specimens was microbially induced carbonate precipitation (MICP), a bio-cementation technique that builds calcium carbonate around silica particles [4].

Specimens of various cementation levels, and hence various combinations of permeability, porosity and strength were tested in a fracture capture apparatus capable of reproducing field conditions.

The experimental behaviour was then examined (i.e., infiltration/fracturing response, fracturing patterns and behaviour) and critical concepts from the field of advanced geomechanics, which have been neglected in numerical studies, such as enhanced permeability, infiltration, flow type, insitu stresses and the elastoplastic behaviour of the material itself are considered to understand the experimental results.

First, dimensional analysis is performed to reveal the role of permeability, flow rate and stress anisotropy in the fluid flow in weakly cemented porous media and then the concept of brittleness index (BI) and cavity expansion theory is applied to the findings [5].

Results show that the fluid flow properties are dominant in fluid flow experiments in such weakly cemented and highly porous media, while the effects of stress levels and anisotropy are also of great importance as the stress dependent brittleness indices provided better fits. Finally, conventional fracture initiation criteria have been proved inadequate in interpreting the findings as the results are better described by the pressure limits derived from the cavity expansion theory.

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HF propagation with Proppant injection using the FEM with zero-thickness interface elements.

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Hydrocarbon recovery from unconventional reservoirs consisting of deep low-permeability rock layers, often relies on the technique of Hydraulic Fracture. In this technique, wells are usually drilled vertically down to the desired depth and then turned 90˚ to a horizontal section which develops within the target layer in the direction perpendicular to the lowest principal stress. It is in this horizontal section that vertical hydraulic fractures are created along planes perpendicular to the well axis. This is achieved by first perforating the well lining and surrounding rock in several directions around the well axis ("cluster"), then installing packers, normally encapsulating a group of clusters at a time ("stage"), and finally injecting the fracturing fluid. In order to maintain the fractures open after the end of the injection, once the fractures have started propagating sand or similar proppant particles may be mixed with the injection fluid. Proppant will then spread over the opening fractures with the intention that it remains as evenly distributed as possible within the fractures. The definition of parameters such as cluster spacing, number of clusters in a stage, distance between wells, injection sequence, duration and intervals of proppant injection, particle sizes, etc. is normally supported by numerical calculations using commercial software fully integrated within the workflow of the O&G industry. However, these tools may be sometimes based on simplifications [1] and often not fully transparent about the underlying asumptions and methodologies.

This motivates the development of in-house codes based on rigurous mechanical principles for solid, fluid and proppant transport in a full 3D environment. In this paper, a model is presented which is based on the FEM with zero-thickness interface ("cohesive") elements, which are pre-inserted along the potential fracture paths. Their mechanical behavior is governed by a fracture-based constitutive model integrating normal (mode I) and shear (mixed mode + frictional) behavior. Fluid flow takes place through the porous continuum, but especially along fractures, the transmissivity of which is drastically affected by opening via the cubic law [2,3]. Proppant transport within the rock mass takes place exclusively along the fractures which are open beyond a threshold related to particle diameter, and is governed by a non-linear advection-diffusion equation, combined with the gravity effect (Stokes deposition velocity). The numerical implementation is based on massive MPI parallelization using PETSC libraries and HDF5 i/o files, with very good scalability.

In the presentation, the main aspects of the model are briefly described, and examples of application are shown including single and multiple fracture with stress shadow interaction. If the clusters are too close, fractures cannot develop freely and show alternate patterns in vertical and horizontal directions. Proppant distributions depend heavily on particle density and size, as well as on proppant injection strategies. The overall model therefore turns out a valuable tool to understand complex field observations and help Engineering design.

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Can a bi-lateral stress jump really arrest the height growth of a hydraulic fracture?

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In certain industrial applications, vertical growth of hydraulic fractures beyond a targeted formation of interest can cause economic loss and pose a risk to environmentally sensitive layers [1]. In addition, when micro hydraulic fracturing is used to measure the minimum in-situ principal stress in the subsurface, the vertical fracture growth can lead to packer bypass, compromising the measurement [2].

In sedimentary formations, the presence of layers of high confining stress above and below the formation of interest is a well-known mechanism for the containment of a hydraulic fracture [3]. As the hydraulic fracture penetrates the region of higher confining stress, the stress intensity factor decreases thus limiting the (fracture)-height growth and promoting the propagation parallel to the layers direction. However, a simple 2D plane strain argument shows that there is a limiting penetration above which the vertical growth can no longer be arrested [4]. This raises the question of whether the vertical growth of an initially radial hydraulic fracture can really be arrested when penetrating the higher stress layers.

We consider the symmetrical scenario of an injection point located at the center of a target formation bounded by two layers with similar properties. We assume that the confining stress in the central layer is lower than in the bounding layers, while the other properties are assumed to be uniform for clarity. Using 3D planar simulations and scaling arguments, we determine under what conditions and for how long a hydraulic fracture driven by a constant injection rate can remain confined between two high-stress boundary layers. We find that true, albeit transient, confinement exists and under two conditions. The first is that the radial fracture must be toughness dominated when reaching the interfaces while the second is that the dimensionless confining stress must be above a given threshold. When these two conditions are fulfilled the radial fracture transitions to a toughness dominated PKN-like fracture (see ref. in [4-5]) for which we develop a new analytical solution following the one derived in [5]. In all other cases, the propagation velocity in the vertical direction is only temporarily reduced, so that the fracture regains its radial footprint at a late stage. We show that no hydraulic fracture can be contained indefinitely by a stress jump. Finally, for the case where the true containment exists, we estimate, both analytically and numerically, how long the fracture remains vertically contained.

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Modelling of natural hydraulic fracturing in sandstone cylinders

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Natural Hydraulic Fractures (NHFs) exist predominantly *in situ*. Compared with Induced Hydraulic Fractures (IHFs), NHFs do not have an increasing but rather experience a decreasing pore pressure in the fracture zone [1]. Numerous studies have been conducted on the interaction between NHFs and IHFs, while rare research has addressed why the former exist and how they grow. This work aims to provide a theoretical basis for their generation and intends to justify the fracture criteria of geomaterials, within the framework of the Theory of Porous Media (TPM) constituted with the phase field method [2, 3].

For this purpose, a numerical model is developed to simulate the natural hydraulic fracturing behavior of sandstone. The numerical test scheme is designed to first model the steady-state flow of deep groundwater within the sandstone (rock), and then the changes in loading conditions at deep subsurface foundations, e. g. during sandstone drilling, where the external vertical load is removed, or e. g. due to tunneling, where the load on the tunnel foundation is significantly reduced under water-saturated conditions. These two states will be modelled using (i) a classical biphasic model and (ii) a biphasic model with an integrated phase-field approach to fracture. From (i), we expect a better understanding of the stress and pressure states occurring *in situ*. From (ii), we intend to justify the failure criteria and estimate material parameters of the TPM phase-field model.

Through this study, permeability was identified as a key parameter for the generation of tensile stresses that would cause fracture or damage within the sandstone via a basic biphasic model [4]. Furthermore, the influence of an important fracture material parameter, the energy release rate, G_c, on the growth of NHFs, was studied. An estimated critical range of $G_c > 110$ N/mm, which does not allow NHFs growth, is given as a reference for future studies. In addition, the growth of NHFs shows a strong dependence on permeability. With higher permeability the material is only damaged and does not produce any fracture, while NHFs tend to grow with lower permeability, even though the external force in both cases remains the same.

The study of NHFs provides relevant insights for engineering practice, e.g. measures to increase either the permeability or the energy release rate of the material in order to avoid excessive fracture growth within geomaterials. The TPM frameworks, along with the phase-field method, can also serve as a powerful tool for engineering practice *in situ*.

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Numerical modeling and simulation of the interaction between hydraulic and natural fractures using high aspect ratio interface elements

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Hydraulic fracturing is a reservoir stimulation technique widely used in the oil industry mainly to induce hydraulic fractures in low permeability reservoirs through the injection of a fluid highly pressurized. Thus, the hydraulic fracture (HF) facilitates the fluid flow in the reservoir. In the cases where the reservoirs have natural fractures (NF), the interaction between the HF and NF can occur in different ways, such as (i) HF directly crossing the NF; (ii) NF blocking the HF propagation; and (iii) NF changing the direction of HF propagation [1].

This is a complex multiphysics problem that involves the coupling of at least three process [2]: (i) the fluid pressure inducing mechanical deformation; (ii) the flow of fluid within the fracture; and (iii) the fracture propagation. In order to overcome this challenging task, this work proposes the use of high aspect ratio interface elements (HAR-IEs) to model the HF formation and propagation as well as its interaction with the NF. The HAR-IEs mechanical behavior is described via an appropriate scalar damage model and the fluid flow behavior is expressed by the classical cubic law [3]. Moreover, these elements are positioned in the finite element mesh according to the Mesh Fragmentation Technique, which allows the HF propagates freely in the domain [4]. The proposed methodology present some advantages to deal with discontinuities in porous media: (i) it is relatively simple to implement HAR-IEs in already existing finite element codes, since they are based on standard elements; (ii) no special integration rules to obtain the internal forces are required; (iii) the analyses are conducted in a completely continuum framework; (iv) tracking algorithms to control the fracture propagation through the domain are not necessary.

The numerical simulations performed in this work studied the scenarios resulting from HF-NF interaction under: (i) different NF apertures; (ii) different approach angles between HF-NF; and (iii) different *in-situ* stress states. Smaller apertures do not influence significantly the HF propagation, since the fluid penetration in the NF is negligible, and in this case, the HF directly crosses the NF. On the other hand, higher apertures affect the HF propagation by changing its preferential direction. The approach angles can affect the HF propagation mainly when they are smaller because the NF represents a path easier to follow than the rock mass. Confinement stresses play another important role in the HF-NF interaction, which enforces HF propagates through the NF (i.e., crossing it). Moreover, the numerical technique proposed in this work proved to be robust, stable, and efficient, since the simulations did not present non-convergence issues and the results agree well with works available in the literature.

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Modeling anisotropic damage using a reconstruction by rational covariants of the elasticity tensor obtained by Discrete Element tests

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When submitted to mechanical loading, quasi-brittle materials such as concrete are degraded. This degradation leads to a decrease in stiffness and a loss of isotropy. In the literature, different anisotropic damage models account for those phenomena. However, anisotropic damage models usually require complex experimental identification procedures.

This study aims at deriving a 2D anisotropic damage model from discrete beam-particle simulations. This work is the continuation of previous studies [1, 2].

A virtual beam-particle [3] unit cell is loaded with multi-axial proportional and non-proportional loadings until failure. Those simulations explicitly represent micro-cracking and describe its impact on the effective elasticity tensor. During the loadings, there are two phases of failure: diffuse nucleation of micro-cracks, which then coalesce as macro-cracks. We construct a dataset of effective elasticity tensors using the measurements during each loading.

The formulation of the anisotropic damage state model is done in two parts. We start by defining a damage variable and then model the effective elasticity tensor from this damage variable using the dataset. To achieve those objectives, we analyze the dataset under the light of two mathematical tools. The first is the (exact) distance to a symmetry class (here, to orthotropy). Using this tool, we show that most of the effective elasticity tensors in the dataset are indeed not isotropic. An anisotropic damage model is therefore required to represent the impact of micro-cracking on the elastic properties. We also show that most tensors are close to being orthotropic, so we next assume that the elasticity tensor is at most orthotropic. The second mathematical tool is the harmonic decomposition of an elasticity tensor coupled with a reconstruction by rational covariants. It decomposes any elasticity tensors into two invariants (shear and bulk modulus), a 2nd-order tensor covariant and a 4th-order tensor covariant. Both covariants are harmonic, i.e., traceless and totally symmetric. This decomposition enables us to introduce a damage variable to recover exactly the bulk modulus and the 2nd-order covariant from the damage variable and initial elastic properties. Then, we propose different models to express the shear modulus and the 4th-order harmonic tensor from damage. Thanks to the orthogonality property of harmonic decomposition terms, the models for each part are independent. This procedure enables us to obtain a satisfying state model requiring the introduction of only one parameter up to high levels of damage.

The damage yield surface associated with the beam-particle is analyzed in the second step. We show that a Drucker-Prager criterion fits the discrete model yield surface. Finally, we propose an evolution model based on invariants of the damage variable.

To summarize, we propose a 2D anisotropic state model that accurately represents the impact of micro-cracking on the effective elastic properties up to a high level of damage. We also propose a damage evolution model. A similar methodology could be applied in the 3D case in future studies. Another perspective is adding the effect of crack closure (with contact and friction).

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Peridynamics for Soil Desiccation Cracking Simulation: Coupled Hygro-mechanical Model, Staggered and Monolithic Solution

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The soil desiccation cracking attributed to moisture loss will significantly weaken the mechanical properties of soil and cause various potential natural disasters. The numerical simulation of soil desiccation cracking remains challenging within the framework of classical continuum mechanics. To avoid the limitation of classical continuum mechanics and corresponding numerical methods, peridynamics has been proposed and developed for dealing with damage accumulation and crack evolution problems.

The hygro-mechanical peridynamic model and numerical method is developed for this classical hygro-mechanical coupled problem. Specifically, a bond-based peridynamic diffusion equation is constructed by using the peridynamic differential operator. In addition, an improved prototype micro-elastic brittle (PMB) model is adopted with high precision attenuation kernel function and discretized micro-modulus. For the numerical implementation, both staggered and monolithic schemes are developed for the coupled hygro-mechanical problem. The direct integration method of explicit dynamics with an artificial damping term is adopted for the staggered scheme. While the matrix equations are assembled and solved in the monolithic scheme with the boundary conditions imposed by Lagrange multiplier method. Furthermore, the method of controlling the maximum number of bond breakage for non-convergence is explored in the monolithic scheme. For modeling of soil drying and cracking, two-dimensional soil rings, and two- and three-dimensional soil strips are simulated and demonstrated. The soil ring model verifies the accuracy of the coupled hygro-mechanical bond-based peridynamic model and reveals the development mechanism of the number of penetrating cracks. The stress distribution and redistribution law are explored, and the curling phenomenon is captured in the soil strip model.

Summarily, the coupled hygro-mechanical peridynamic model provides a potential strategy in soil desiccation cracking investigation for real-scale simulation and fine mechanism exploration.

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Damage growth in coal under uniaxial compression

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Quantitative analyses of damage growth during in-situ uniaxial compression are significant to understand fracture and permeability in coal. Given the influence of complex microstructures and pre-existing cracks, it is difficult to quantify damage processes when based upon X-ray microtomography alone. Therefore, an advanced finite element based digital volume correlation (DVC) algorithm is proposed, in which mechanical regularization, damage law, and mesh refinement schemes were considered simultaneously to allow for the measurement of kinematic fields in cracked regions with very fine spatial resolutions. In particular, damage was quantitatively characterized even at levels less than one voxel by estimating crack closure/opening displacement fields of pre-existing/newborn cracks.

The implemented procedure consists of the following four steps.

1. Mechanical regularization based on the equilibrium gap method is introduced into FE-based global DVC as a low-pass filter to dampens out high spatial frequencies, theryby gaining an initial estimation of kinematic fields for which linear elasiticy applies.
2. A brittle damage law [1] was added in the above regularized DVC framework to allow for high displacement gradients in cracked zones. Specifically, a damage variable was applied to reduce the regularization weight of damaged elements that are detected by gray level residuals and maximum principal strains.
3. A mesh refinement scheme was carried out in those damaged elements to better capture crack shapes and kinematic characteristics. A master-slave elimination was utilized to deal with hanging nodes at the junction of coarse and fine meshes. In addition, the mesh size is no longer limited thanks to regularzition, which can even reach the voxel level if needed.
4. All the workflow was integrated into a multimesh DVC [2] scheme to measure internal deformation fields and evaluate crack opening and closure displacement fields. Such information is very useful to understand the damage scenario in the studied experiment.

In the investigated uniaxial compression, damage mechanisms of coal were quantitatively studied based on the initiation and propagation of newborn cracks, as well as the closure of pre-existing cracks. The measurement uncertainty of multimesh DVC was assessed based on the first two scans. Before levels equal to 50% of the ultimate strength, only pre-existing cracks closed. When loaded to 60% of the ultimate strength, microcracks initiated at the end of the pre-existing cracks, then further opened and propagated vertically. Such interactions among pre-existing and newborn cracks explained the damage development process from subvoxel to voxel levels. This study demonstrates the potential of regularized multimesh DVC for damage quantification in quasi-brittle materials using very small spatial resolutions.

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Parameter calibration of a fibre-reinforced concrete fracture model by means of co-simulation between OOFEM and Scipy

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The use of fibre-reinforced concrete (FRC) is not new, but has experienced a big impulse in recent years. The increasing interest in FRC has produced a remarkable number of experimental studies to identify how diverse aspects of their production affect their properties, both in fresh state and hardened. Together with these experimental studies, several approaches have been proposed for numerically reproducing fracture in FRC. It is worth mentioning the use of cohesive fracture by using a trilinear softening diagram [1] that allows reproducing the behaviour of this material taking into account different FRC mixes (with different fibre length and proportion), different loading scenarios [2] and capturing the size effect [3]. Moreover, the trilinear softening diagram is defined with crack opening and stress values that are related with physical parameters of the FRC mix (concrete strength, fibre length, polymer elastic modulus or the fibre proportion, for instance).

The trilinear softening diagram is defined by six values (f_t, f_k, f_r, w_k, w_r and w_f), that correspond to stresses (f_i) and crack opening values (w_i) that must be calibrated to fit the experimental results. Since this process includes a relatively high number of parameters to adjust, it implies carrying out a trial and error process that may lead to a high number of models to be run (typically, around 25 would be a fair estimation).

The trilinear softening diagram has been successfully used with an embedded fracture model in the past. In this study, the trilinear softening diagram is adapted and implemented in a smeared crack model of the free finite element code OOFEM [4] and the calibration process of the parameters that define the trilinear softening diagram is carried out by means of an algorithm that makes use of an optimization package of Scipy [5]. To illustrate the performance of this algorithm, an experimental reference of a three-point bending test is used and, by providing the experimental load-displacement diagram and an initial set of parameter values, the algorithm is able to provide a set that minimizes the deviation of the numerical model with respect to the experimental curve. Error is computed as the difference between the experimental and the numerical results at selected points of the load-displacement diagram.

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Minisymposium RFM:

Regularized failure models: Phase-field and other models

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

Griffith criterion for phase field fracture

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We provide a phase-field version of Griffith's criterion [4] and show that it is satisfied by the evolution obtained from the staggered scheme, both in continuum and in finite element settings [1].
We employ the second order Ambrosio-Tortorelli approximation of the Griffith's energy, $AT_2(u, v)$, that is defined as the sum of the phase-field elastic energy $\mathcal{E}(u, v)$ and of the dissipated energy $G_c\mathcal{L}(v)$, where $\mathcal{L}(v)$ is the phase-field approximation of the crack length. We introduce a notion of *phase-field energy release* $\mathcal{G}(v)$.
We consider a quasi-static evolution in a time interval $[0, T]$. The irreversibility of the crack is modeled by the monotonicity of the phase field variable v. This hypothesis does not directly imply the thermodynamic consistency of the dissipated energy, therefore we require that $\dot{\mathcal{L}}(v(t)) \geq 0$.
The Griffith's criterion in phase-field setting is written in terms of the following Karush-Kuhn-Tucker conditions: $\mathcal{G}(t, v(t)) \leq G_c$ and $(\mathcal{G}(t, v(t)) - G_c)\,\dot{\mathcal{L}}(v(t)) = 0$.
The evolutions are obtained by *staggered (alternate) minimization* for the energy AT_2, where we require monotonicity of the phase-field variable in time and not over each iteration as in [2]. The time interval $[0, T]$ is discretized and at each time step t_k the solutions u_k and v_k are defined as the result of the staggered minimization scheme, flanked by a stopping criterion and a constraint on the numer of iterations.
Passing to the limit as the time step approaches zero we find an evolution $t \mapsto (u(t), v(t))$ such that in the steady-state regime:

- $(u(t), v(t))$ is an equilibrium point for the energy $AT_2(\cdot, \cdot)$;
- $v(t)$ satisfies the Griffith's criterion and the thermodynamical consistency;
- an energy balance identity holds.

Obviously the evolution may depend on the discrete scheme and may present also unstable regimes, where propagation is catastrophic and Griffith criterion does not hold.
Analogously, if we discretize the domain with finite elements, the limit evolution as the time step approaches zero satisfies all the properties listed above.

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A Crack Nucleation Scheme for the Phase Field Approach to Brittle Fracture

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Due to the polyconvexity of the phase field formulation for fracture, starting from a crackless solid, a standard Newton iteration may lead to a solution with no crack, even though a cracked solution has a lower total energy. As such, the critical load for cracking is highly overestimated. Here, we propose an algorithm termed "parallel universe" algorithm to capture the global minimum. This algorithm has two key ingredients: (a) a necessary condition for cracking solely based on the current crackless solution, and (b) beginning from when this condition is met, Newton iteration with two initial guesses, a crackles one and a cracked one, will both be performed and the converged candidate solution with lower energy is accepted as the solution at that load step. Once the cracked candidate solution is accepted, the crackless one is discarded, i.e., only one universe is retained. This cracked initial guess is obtained only once for all load steps by solving a series of similar minimization problems with a progressively reduced critical crack energy release rate. Numerical examples with isotropic and anisotropic critical crack energy release rates indicate that the proposed algorithm is more reliable (as there is no need to retrace) and more efficient than the standard Newton iteration and a well-known backtracking algorithm. More details can be found in [1].

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Revisiting Size Scale Effects in Phase-field

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The study of size scale effects on fracture in materials science is a complex and ongoing challenge. Despite numerous advances in computational modeling, there is still much to be learned about how the size and shape of a material influences its fracture behavior. This is a critical area of research, as a thorough understanding of size scale effects is essential for accurately predicting and improving the mechanical properties of materials. As noted by Bazant, "If scaling is not understood, the theory itself is not understood" [1]. With the recent development of phase field theory, there is a renewed focus on understanding the size effects on fracture and how they impact material behavior.

This research introduces a geometrical scaling framework to capture the geometric transformation relationship between material models and scaling. The framework utilizes a scaling matrix that defines the transformation between the original and scaled domains and adjusts the gradient operator accordingly without loosing variational formulation, allowing it to handle various scaling scenarios including lateral expansion, horizontal expansion, symmetric scaling, and rotations. The proposed framework has been applied to AT1, AT2 [3], and PFCZM [4] models and has been successful in mimicking the original and scaled models without the need for additional model development or computational resources. The model is solved using both variational inequality (fenicsx) and ABAQUS (UEL) to ensure unbiased results. Furthermore, the model has the ability to recover size scale laws and structural bifurcations with constant computational time for any scaling within the framework. Moreover, mesh issues concerning phase field are addressed.

As an example, a plate with a notch is studied using a scaled model of dimension (1×1) to represent the results of the original model $(x \times y)$. Figure 1a shows the scaling of the symmetrical model while Figure 1b presents the lateral and horizontal scaling on the AT2 model, with a comparison between the scaled and original models.

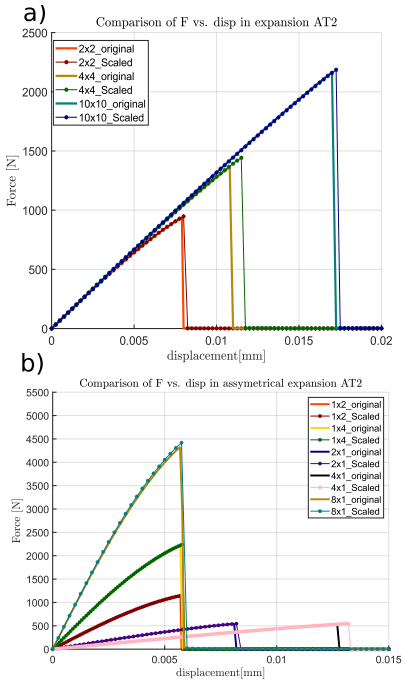

Figure 1: a) Comparison of Symmetrical, and b) asymmetrical loading on AT2 model with scaled and original model [2].

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An enhanced phase field approach to cohesive fracture

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Cohesive zone models show great potential for handling non-linear fracture mechanics. In contrast to brittle fracture models, cohesive fracture models include an interface energy not only depending on the geometry of the crack, but also on its opening. The opening of the crack is mathematically defined as displacement jump $[\![\boldsymbol{u}]\!]$. The dependence of the interface energy on the displacement jump results in tractions across the crack, which can be described by a so-called traction-separation-law $\boldsymbol{t}([\![\boldsymbol{u}]\!])$. The probably two most important physical material properties of traction separation laws are the strength of the material and the fracture energy.

As far as the finite element implementation is concerned, several techniques have been proposed for incorporating cohesive fracture laws. The first class of those techniques are based on discrete interfaces — either between bulk elements or within bulk elements (XFEM). The second class of techniques employs diffuse interfaces with a finite thickness such as phase field models. The major advantage of this type of models are the easy tracking of the (evolving) crack geometries.

A promising phase field approach to cohesive fracture was recently introduced by Conti et al. [1] and further investigated by Freddi and Iurlano [2]. For thus framework, Γ-Convergence to a cohesive fracture models was rigorously proven. Within this talk, the model proposed in [1, 2] will be extended with respect to:

- a geometrically exact setting,
- arbitrary hyperelastic material models,
- independent material parameters for the bulk material and the interface (including the strength and the fracture energy of the interfaces)
- the introduction of the Microcrack-Closure-Reopening (MCR) effect (cracks only evolve under tensile stresses)

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Coupling of phase-field based fracture propagation with healing in self-healing materials

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Self-healing materials exhibit damage tolerance as they can recover from mechanical damage either due to their natural ability or by certain material constituents acting as healing agents. Experimental investigations on self-healing material has been an active area of research over the last few decades with the development of extrinsic self-healing mechanisms, such as micro-capsules, vascular structures, and shape memory alloys/polymers [1]. Various models for prediction of mechanical behaviour, capturing the damage and healing, have been developed based on the continuum damage mechanics, micromechanics, and cohesive zone modelling [2, 3].

Damage mechanics based damage-healing models are developed at the macroscopic continuum scale, which track the evolution of damage and healing as internal state variables and correspondingly evaluate the degradation and recovery in the material integrity. Damage (D_g) and healing (h_l) variables are defined as fraction of the total area that has undergone damage, and the fraction of the damaged area that has undergone healing, respectively [2]. The collective influence of damage and healing on the material's constitutive response is given by the effective damage variable defined as $\phi_{eff} = D_g\,(1 - h_l)$ [2]. Phase-field based damage modelling is a diffusive damage approach which, unlike damage mechanics, enables tracking individual cracks while also avoiding an explicit representation of kinematic discontinuities.

The objective of present work is to develop a coupled phase-field-based damage - healing model for the analysis of crack propagation in self-healing material. An elastic self-healing material, undergoing small deformation with a pre-existing crack (not necessary requirement), is considered in the present work. The minimization of total potential energy of system (bulk elastic and crack surface energies) provides the governing equations for the phase-field damage model [4]. A quadratic energy degradation function is considered, and tension-compression split of elastic strain energy is performed such that damage variable evolution is driven by tensile elastic energy (no damage in compression). The healing evolution is proposed accounting for both, stress-based and stress-free, cases.

The primary focus of present work is on development of staggered solution scheme to estimate damage-healing evolution and track fracture path for each loading increment. The phase-field equation is firstly solved based on the initial definitions of displacement, phase-field, and history variables. The equilibrium equation, coupled with the healing evolution equation, is secondly solved based on the updated phase-field parameter for the current loading increment. The numerical implementation is performed by meshless local differential quadrature method, and various boundary value problems are solved illustrating the healing of multiple cracks, non-local healing evolution, fracture propagation coupling the damage and healing, and stress-free healing.

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Multi-axial loadings in phase field model of fracture: Part 1

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Phase field modeling of fracture is gaining popularity in the fracture mechanics community, particularly for its ability to generate cracks with arbitrarily complex geometries and topologies in two and three dimensions without the need for ad hoc criteria. The model first introduced in [1] has a clear connection with Griffith's propagation criterion via Gamma convergence tools and further results [2] have shown that, in addition to propagation, it can quantitatively predict crack nucleation for mode-I loading. However, the initial model cannot reproduce with flexibility the experimentally measured strengths under multiaxial loads. Moreover, a modification is necessary to avoid the interpenetration of crack surfaces in compression and reflect the physical asymmetry of fracture behavior between tension and compression [3]. New models are often validated through different case studies that show specific potentials, making their comparison not immediate and analysis of limitations not straightforward. Among these contributions, some preserve the variational nature of the phase field model [3, 4, 5, 6] while others seek flexibility by stepping outside the variational framework [7]. The most popular variational solutions [3, 4] are based on elastic energy decompositions. This idea is adopted in [5, 6], justified through structured deformation theory.

In this first part, we present a study that sorts the wealth of literature based on specific criteria. We define these criteria as the ability to flexibly reproduce multiaxial strength and avoid interpenetration of crack faces, and so we perform a systematic review of some available models. Based on these concepts, we propose numerical benchmarks to evaluate the behavior of solutions in literature. In particular, the proposed tests provide an assessment of a phase field model for both nucleation and propagation.

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Multi-axial loadings in phase field model of fracture: Part 2

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Phase field modeling of fracture is gaining popularity in the fracture mechanics community, particularly for its ability to generate cracks with arbitrarily complex geometries and topologies in two and three dimensions without the need for ad hoc criteria. The model first introduced in [1] has a clear connection with Griffith's propagation criterion via Gamma convergence tools and further results [2] have shown that, in addition to propagation, it can quantitatively predict crack nucleation for mode-I loading. However, the initial model cannot reproduce with flexibility the experimentally measured strengths under multiaxial loads. Moreover, a modification is necessary to avoid the interpenetration of crack surfaces in compression and reflect the physical asymmetry of fracture behavior between tension and compression [3]. New models are often validated through different case studies that show specific potentials, making their comparison not immediate and analysis of limitations not straightforward. Among these contributions, some preserve the variational nature of the phase field model [3, 4, 5, 6] while others seek flexibility by stepping outside the variational framework [7]. The most popular variational solutions [3, 4] are based on elastic energy decompositions. This idea is adopted in [5, 6], justified through structured deformation theory.

In light of the criteria defined in the first part of the presentation, we examine the influence of different softening laws on the volumetric and deviatoric components of the strain energy density. We then evaluate a new model that is based on distinctive volumetric-deviatoric softening behaviors, using the benchmarks established in the previous part of the study.

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An experimental study of crack growth under compression using a Phase-field theory

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Phase-field theories have gained a great deal of attention in recent years for their application to numerically modeling fracture. While phase-field theories have many advantages, one that stands out is that the crack mechanics are inherently derived from a minimization framework that couples strain and fracture energies. It is, however, necessary to decompose the strain energy density into tensile and compressive components in order to prevent interpenetration of crack surfaces and to select crack paths that are physically trustworthy. Spectral decompositions [1] and hydrostatic-deviatoric decompositions [2] are among the most popular methods of decomposing the strain energy density. Both of these decomposition techniques have a number of disadvantages, the most significant being that neither is able to adequately handle crack growth in compression [3]. There have been several attempts made to address this issue through the development of alternative decomposition schemes for the simulation of fracture under compression cf. [4,5]. There is, however, a drawback to these models, which is the fact that as a crack develops, stiffness may remain with a fully developed crack subjected to a shear load. Recently a model has been proposed to circumvent this problem by presenting a modified strain energy decomposition that is a combination of spectral and hydrostatic-deviatoric decompositions and is inspired by the classical Mohr-Coulomb fracture criterion [6]. In this study, this model is tested against a series of compressive tests in order to demonstrate its capability to predict the crack paths. The tests were conducted on specimens made of gypsum plaster which contained multiple embedded flaws and holes. The numerical results with a unique set of material parameters have been compared to experimental data both in terms of crack pattern and loading curve and they were in good agreement showing that the model is providing mechanistic insight into the fracture of brittle materials.

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A phase-field and interface damage model for mixed-mode fracture in materials with inclusions

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The presented approach provides a tool for analysing fracture in materials and along material interfaces of general multi-domain structures under quasi-static conditions. It is intended for materials appearing in engineering structures made of multiple components: including grains or fibres which may be spaced inside the matrix material. Description of the fracture processes are based on considering internal parameters in sense of damage.

Two independent parameters are introduced to make a difference between interface and material cracks. The state of interface faults is defined considering it as a thin adhesive layer and pertinent internal variable renders relation between stress and strain quantities in the form known in cohesive zone models. Such treatment results from problems of delamination [1] or adhesive contact [2] which introduced requested internal variable for interface damage. The other parameter is defined in bulk domains and controls the degradation state in a sense of phase-field fracture guaranteeing the damaged zones in form of smeared cracks. Though originally considered as a regularisation of variational Griffith-like models of fracture [3], the phase-field appriach developed to a powerful computational tool, which my modify damaging behaviour by adjusting material degradation, fault initiation [4], or even be combined with flaws related to material interfaces [5]. Another important feature of modelling both interface and phase-field rupture is the capability of making difference between fracture modes which is useful when the structure is exposed to combined loading causing both tensional and shear effects. It is usually related to additional dissipation in other than opening fracture modes. The crack mode sensitivity was in this sense described by the model in [1] and an appropriate phase field model can be found in [6]. The present contribution intends to integrate both concepts as it was sketched by the author in [7].

The computational techniques used in the approach utilise possibility of defining the solved problem variationally which allows implementation of (sequential) quadratic programming methods into a finite element discretisation and appropriate time stepping methods. The MATLAB simulations with an in-house computer code validate developed formulation for analysis of fracture problems in multi-domain elements of structures.

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Modeling mixed-mode fracture in elastomers at finite strain

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Elastomers are widely applied in automobile industry for rubber tires and tubes. At large deformations, they behave elastically, and the fracture phenomenon is nonlinear. Therefore, mode decomposition is not possible as in the case of linear elastic fracture mechanics [LEFM]. Understanding fracture mechanism in elastomers under mixed-mode conditions is necessary. Recently, experimental studies are conducted on mixed-mode crack propagation in silicone elastomers [1]. The crack propagation for different degrees of mode mixity is reported. Computational modeling helps in studying the effect of mode mixity on mechanical and fracture response of elastomers. Phase field approach is one of the popular methods to model fracture in cracking solids. It has been developed using variational approaches [2]. The total potential energy is minimized to obtain the displacement field and crack phase field using a staggered approach. This approach has been adopted to model fracture in isotropic [3], anisotropic [4], and hyperelastic [5] materials. Mixed-mode fracture criteria can be incorporated into the crack evolution equation using a power law [6]. A thermodynamically consistent phase field formulation for modeling mixed-mode fracture in elastomers is presented. To model elastomers, a nearly incompressible hyperelastic material model is adopted. To model the mixed-mode fracture, a volumetric-deviatoric split is considered, and to ensure the crack doesn't heal, a tension-compression split of the strain energy is also considered. Mixed-mode critical energy release rate is introduced into the crack driving force. A mixed-mode test is conducted on silicone elastomers similar to the material used in experiments in [1]. By varying the degree of mode mixity, the crack angles and mechanical response of the material are plotted. The obtained results are compared with the experimental investigations.

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2D phase-field ductile fracture modeling in orthotropic paperboard materials

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Driven by growing online shopping habits and demand for recyclable packages, the global carton packaging market is rapidly expanding. In the case of food packaging, to match the more and more restrictive regulations on recyclability and waste reduction, carton packaging manufacturers have to use thinner and lighter weight grades of carton board, reducing at the same time the use of polymeric or aluminum coatings, without compromising safety and quality of the packaging. The combination of growing competition and more severe regulations is forcing the packaging companies to search for new designs and innovative solutions, where the structural behavior of the paperboard material plays a key role, since it provides the mechanical strength to the final product.

The present work is devoted to the phase-field simulation of crack propagation in paperboard. Paperboard is a strongly orthotropic material: Machine Direction (MD) and Cross-machine Direction (MD) are the in-plane directions, whereas ZD denotes the thickness direction. MD and CD mechanical properties are in general up to two orders of magnitude higher than in ZD. While large strains and damages are associated to out-of-plane deformations, in-plane fractures are usually associated to small strains. As an initial step towards the modeling of crack propagation in paperboard under arbitrary loading conditions, the present work is restricted to small-strain, in-plane crack propagation.

Very accurate orthotropic elastoplastic models for paperboard are available in the literature (see, e.g., [1, 2]). However, a reliable model for the description of coupled ductile elastoplastic and brittle damage mechanisms in paperboard is still missing. The objective of the present contribution is therefore to propose a phase-field model of in-plane (MD-CD) crack evolution in paperboard.

A variational, finite-step formulation for elastoplastic solids, based on a backward-Euler return mapping scheme, is taken as starting point for a variational formulation of ductile fracture. The energy functional is enriched with a phase-field damage-like variable and with its gradient, following the phase-field approach to brittle fracture. An AT1 model is used, guaranteeing in this way the presence of a purely elastoplastic regime in the material response. An effective stress description, with plasticity developing only in the continuous (undamaged) part of the material, is adopted. The damage activation criterion is modified by the addition of a non-variational term to account for the plasticity-driven nature of crack evolution and for the orthotropic behavior of paperboard. The purpose of this function, depending on a scalar measure of accumulated plastic strains, is to modulate the competition between plastic and fracture dissipation mechanisms in the crack nucleation phase and their interaction in the subsequent crack propagation. Unlike in standard approaches to orthotropic phase-field formulation, the orthotropic nature of the material is accounted for without considering an additional damage variable or introducing a structural tensor in the gradient damage term. Rather, the scalar measure of plastic evolution in the modulation function is chosen to depend in a different way on the plastic strains developed in the different material orthotropy directions.

The proposed model is validated against experimental results and its predictability is assessed. While only the application to paperboard has been studied, the model is general and the same approach could be considered for the modeling of other orthotropic elastoplastic materials.

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Variational formulation with dissipation-gradient regularization for softening plasticity models

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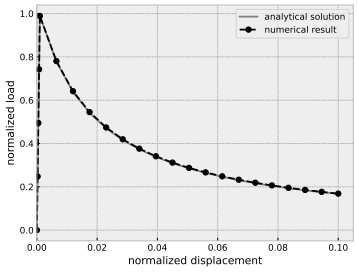
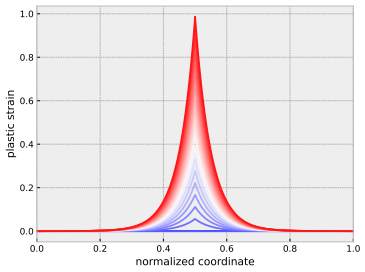
Constitutive plasticity models with softening effects require a regularization framework to describe strain localization in an objective way. One broad class of methods uses gradient theory, which includes both strain-gradient models and models with gradients of internal variables. In most cases, gradient terms are included as an additional contribution to the free-energy potential. However, these models have been shown to exhibit undesirable properties such as unlimited spreading of localization bands in later stages of the softening process [1, 2]. Alternatively, one may modify the expression of the dissipation potential by introducing additional gradient terms, as has been proposed to model size-dependent strengthening behavior of metals in agreement with micron-scale tests [3, 4]. To our knowledge, this strategy has not been explored for dealing with softening, and it is the focus of our work. We propose regularization of softening plasticity models obeying the normality rule using the gradient of the plastic strain increment in the dissipation potential, followed by an incremental variational formulation. We solve the corresponding optimization problem using dedicated algorithms for convex variational problems represented as discrete conic programs. We carry out numerical finite element simulations in one and two-dimensional settings, using nonlinear softening laws for von Mises plasticity. These examples illustrate the emergence and development of localization bands. Our contribution shows that the band width is bounded even in the vicinity of the ultimate state. Finally, we compare the numerical results with analytical solutions to support the well-posedness of both our dissipation-gradient regularization and its computational treatment.



(a)



(b)

Figure 1: Bar under traction after [1]. (a): Load-displacement responses. (b): Plastic strain profiles.

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A variational damage-plasticity model depending on hydrostatic stresses

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Ductile fracture is characterised by large plastic strains before a macroscopic crack occurs. Complex processes in the material such as void nucleation, coalescence and growth leading to plastic slip lines and shear bands need to be considered. To capture these characteristics, various local plasticity models have been proposed and extensively used, such as the Gurson-Tvergaard-Needleman (GTN) model.

However, the GTN plasticity model is not well-defined when it comes to the localisation of porosity, as this coincides with the loss of ellipticity of the incremental equilibrium equations. This leads to mesh dependence in FE simulations, which can be eliminated by a non-local regularisation. This has been achieved using an integral condition for the porosity [1], [2] or introducing the gradient of the equivalent plastic strain [3]. The latter method requires an extended associated flow rule since the plastic flow can become singular due to the gradient plasticity term. Alternatively, the coupling of local GTN plasticity with a phase-field model has been proposed [4]. In this case, the phase-field is regularised, but the porosity may still localise and lead to mesh sensitivity, again requiring the introduction of gradient plasticity.

In this work, we suggest a coupled gradient damage (phase-field)-plasticity model that can handle von Mises plasticity as well as more advanced plasticity models to reproduce phenomenological aspects of ductile fracture. The proposed model is variationally consistent, i.e. the equilibrium and damage evolution equations stem from an incremental energy minimisation principle. The plastic dissipation depends on both the deviatoric and the hydrostatic components of the plastic strain tensor. Localisation is prevented by regularisation through the gradient of the damage (phase-field) variable. The resulting model is able to reproduce a material behaviour similar to that of the GTN model with no need of directly introducing the porosity as additional variable and with no need for gradient regularization of the plasticity model.

The behaviour of the proposed model is studied with several benchmark tests. Their results are compared with the results from GTN porous plasticity coupled with a phase-field model.

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Moving layers and graded damage coupling with elasto-plasticity

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The paper investigate the coupling between graded damage [1] and elasto-plasticity. The elastic properties $\mathbb{C}$ of the material depends on a damage variable d, then the free energy w depends on the strain ε, on internal variables α and on damage d:

$$w = w(\varepsilon, \alpha, \mathrm{d}).$$

Damage variable is bounded and its gradient is bounded by a concave function $f(\mathrm{d})$ in order to limit its concentration:

$$g_2(\mathrm{d}) = ||\nabla \mathrm{d}|| - \mathrm{f(d)} \leq 0, \quad \mathrm{f}(0) > 0.$$

These two conditions are taken into account by two Lagrange multipliers μ_i

$$\mu_i \geq 0, \quad g_1 = \mathrm{d}(\mathrm{d}-1) \leq 0, \quad \mathrm{g}_2 \leq 0,$$
$$\mu_1 g_1(\mathrm{d}) + \mu_2 \mathrm{g}_2(\mathrm{d}) = 0.$$

Introducing the potential energy $\mathcal{E}$ of a body Ω submitted to prescribed displacement on $\partial\Omega_u$ and tension on the complementary part $\partial\Omega_T$.

$$\mathcal{E}(u, \alpha, \mathrm{d}, \mu_\mathrm{i}) = \int_\Omega w(\varepsilon(u), \alpha \mathrm{d}) \mathrm{d}\Omega + \int_\Omega \mu_i g_i(\mathrm{d}) \mathrm{d}\Omega - \int_{\partial\Omega_\mathrm{t}} \mathrm{T}^\mathrm{d}.\mathrm{udS}$$

The evolution of the internal parameter (α, d) are given by normality laws

$$\dot{\alpha} = \lambda \frac{\partial \Phi}{\partial A}, \lambda \geq 0, \Phi(A) \leq 0, \lambda\Phi = 0$$
$$\dot{\mathrm{d}} \geq 0, Y - Y_c \leq 0, \dot{\mathrm{d}}(Y - Y_c) = 0$$

where Φ is a convex function of the thermodynamical force A associated to α :$A = -\dfrac{\partial \mathcal{E}}{\partial \alpha}$, and Y_c is a critical value for local fracture, Y is the release rate of energy associated to damage evolution, $Y = -\dfrac{\partial \mathcal{E}}{\partial \mathrm{d}}$.

The variations of potential energy gives the driven forces:

$$A = -\frac{\partial w}{\partial \alpha},$$
$$Y = -\frac{\partial w}{\partial \mathrm{d}} + \frac{1}{f}\, div(\mu_2 \nabla \mathrm{d}) + \mu_1(1 - 2\mathrm{d})$$

Variations of potential energy exhibit discontinuities along the boundary between sound and damaged material, this fact must be discuss.

In particular, w can be discontinuous along moving boundaries, especially along the surface where $\mathrm{d} = 0^+$. If such a discontinuity exists additional dissipation occurs, if not this imposes some continuity conditions on the internal variable α. In this case, in the damaged zone plasticity and damage cannot evolve simultaneously as shown in [2].

This fact is illustrated on analytical examples based on cylindrical or spherical geometries on elasto-plasticity with or without linear hardening.

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Strain localization in elasto-plastic beams based on a phase-field approach

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Structures composed of strain softening materials are prone to failure because of strain localization in relative small critical zones. As loads increase, structures develop localization bands with thin thicknesses, which can be physically separated from the rest of the volume by interfaces. The strain rate becomes discontinuous in correspondence with the band.
It is also possible that strain localization occur in some structures that exhibit perfect plastic behavior as a result of a non-uniform distribution of forces inside them. This can be the case of a beam subjected to a non uniform distribution of the bending moment such that the inelastic curvature develops along the beam axis in a portion that contains a critical section, i.e. the section that experiences maximum bending moment. As the loading process continues, the critical section becomes fully plasticized, the curvature in the same section becomes discontinuous, and the so-called plastic hinge is formed.

As a result of the introduction of the ultimate limit state concept into several building codes for framed structures, engineers began to apply nonlinear structural analysis to these kinds of structures under static and dynamic conditions. Specifically, the nonlinear static analysis method, called *pushover* became very popular due to its ability to provide relevant information, including limit loads, displacement capacities, and overall ductility at an acceptable computational cost. In terms of the assessment of existing structures, this tool is particularly useful since it can be used to identify areas of potential weakness prior to the development of a rehabilitation plan.
The nonlinear finite element analysis can be performed assuming a distributed or lumped plasticity model for the beam element. In the distributed plasticity model, inelastic responses are diffused along a part of the beam whose lenght is comparable to the element length. The response of the element is determined by weighting the behavior at fixed sections, whose number and location are defined by the quadrature rule for numerical integration. The constitutive behaviour of the cross section is either formulated in accordance with classical plasticity theory in terms of stresses and strain resultants [1] or is explicitly derived by discretization of the cross section into fibers [2].
The present work is devoted to the implementation, in a finite element environment, of an elastoplastic Euler–Bernoulli beam element showing possible slope discontinuities at any position along the beam span, in the framework of a modified lumped plasticity. The theoretical treatment of the problem has been developed in a classical way making use of the principles of thermodynamics.
The strain jump at the fully plasticized section is regularized, i.e. smeared along the beam span, taking into account the length of the plastic hinge. This regularization is performed according to the phase-field approach presented in [3]. With respect to other phase-field models, the novelty consists in the homogenization of the inelastic strains through a weak Dirac delta function which, for a multi-axial problem, takes the shape of the Mumford-Shah functional.

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hase field modeling of brittle fracture in large-deformation solid shells with the efficient quasi-Newton solution and global-local approach

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To efficiently predict the crack propagation in thin-walled structures, a global-local approach for phase field modeling using large-deformation solid shell element formulation considering the enhanced assumed strain (EAS) and assumed natural strain (ANS) methods for the alleviation of locking effects is developed in this work.

Aiming at tackling the poor convergence performance of standard Newton schemes, a quasi-Newton (QN) scheme is proposed for the solution of coupled governing equations with enhanced assumed strain shell formulation in a monolithic manner. The excellent convergence performance of this QN monolithic scheme for the multi-field shell formulation is demonstrated through several paradigmatic boundary value problems, including single edge notched shear, fracture of cylindrical structure under mixed loading. Compared with the popular alternating minimization (AM) or staggered solution scheme, it is also found that the QN monolithic solution scheme for the phase field modeling using enhanced strain shell formulation is very efficient without the loss of robustness, and significant computational gains are observed in all the numerical examples.

In addition, to further reduce the computational cost in fracture modeling of large-scale thin-walled structures, a specific global-local phase field approach for solid shell elements in the 3D setting is proposed, in which the full displacement-phase field problem is considered at the local level, while addressing only elastic problem at the global level. Its capability is demonstrated by the modeling of thin-walled photovoltaic laminate under three point bending, which can be appealing to industrial applications.

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Accurate modeling of the fracture of plates using the phase-field method

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Since the last decade, the phase-field method has been increasingly developed [1]. This is due mainly to its good performance in capturing localized plasticity and damage in mechanical structures. The nonlocal nature of the phase-field method [2, 4, 5] is a key to its success in analyzing the damage and fracture propagation without dependency on the mesh size.

This work proposes a new numerical technique based on a strong coupling of damage and kinematics variables for the damage analysis of thin shell structures. To this purpose, the 4-node MITC4 shell element has been developed. It uses six kinematics variables per node (three translations and three rotations) and one extra degree of freedom representing the damage. The developed approach is based on the variational phase-field method proposed by Ambrosio and Tortorelli [3] and adapted to brittle fracture [2]. The condition of damage irreversibility was forced at each step using the penalty technique, not only for its simplicity but also for its effectiveness because it does not increase the size of the problem. The proposed technique has shown to be effective in solving several numerical applications involving thin and thick shell structures, including transverse shear with and without initial cracks. The results were compared to those from the literature using other numerical techniques such as XFEM and the Peridynamics, as well as some experimental results.

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A unified strategy to mitigate the surface effect and to impose in a local way the boundary conditions in Peridynamics models

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Peridynamics is a non-local continuum theory which, thanks to the integral formulation, allows discontinuities such as cracks to initiate and propagate in solids [1]. Due to the non-local nature of the theory, peridynamic models suffer from two interrelated problems at the boundary of the domain: the "surface effect" and a difficulty in imposing the (non-local) boundary conditions. Points close to the boundary are characterised by an incomplete neighbourhood. Consequently, the most external layer of the body shows different material properties with respect to the bulk of the body resulting in an unrealistic variation of the stiffness properties. This phenomenon is known as the "surface effect" [2]. Two main approaches are used to correct it: the definition of modified bonds in the external layers of the domain or the introduction of a fictitious layer of nodes around the domain boundary [2]. Similarly, the imposition of boundary conditions is often achieved using a fictitious layer, in the case of displacement boundary conditions, or by the distribution of the external tractions as body forces applied to a certain number of nodes at or near the boundary. However, there is no general agreement on the way in which the boundary loads or displacements should be "distributed" over a finite number of layers.

We propose a unified and effective method to mitigate the surface effect and properly impose the boundary conditions [3,4]. Introducing a fictitious layer around the body provides the missing nodes, (the fictitious nodes), then multiple Taylor series expansions are used to determine their displacements as a function of the displacements of the nearest real nodes. As a result, the fictitious layer continues to deform as an outer layer of the body, significantly reducing the surface effect.

Furthermore, we introduce a new type of nodes lying on the external surface of the body, the surface nodes [5]. These nodes represent the interactions between the nodes within the body and the fictitious nodes surrounding the body. The equations of surface nodes are defined based on the concept of force flux.

Thanks to this fact, the boundary conditions can be applied directly to the surface nodes, as one would do in a local model. The accuracy of the proposed approach is assessed by means of several numerical examples (1D, 2D and 3D cases) for a state-based peridynamic model: the results are significantly improved with respect to the peridynamic model with no corrections.

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A locally adaptive phase-field model that tracks sharp cracks

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Various adaptive phase-field models of fracture have been proposed recently [1]. Our adaptive refinement strategy [2] is based on considering only two types of elements in a fixed background mesh: h-refined elements along cracks, where a higher spatial resolution is needed, and standard elements in the rest of the domain. The strategy is specifically designed to avoid remeshing, transition elements or the handling of hanging nodes. Continuity of the displacement and damage fields in the non-conformal interface between adjacent elements of different type is imposed in weak form by means of Nitsche's method. This weak imposition of continuity leads to a very local refinement in a simple way: no tuning of Nitsche's parameter is required. The robustness of the approach is illustrated by several examples, including branching and merging of multiple cracks in 2D, and twisting cracks in 3D.

This adaptive phase-field approach is the starting point for a continuous-discontinuous model of fracture [3]. The phase-field equations are solved only in small subdomains around crack tips to determine propagation. With computational cost in mind, an XFEM discretization is used behind the tips to represent sharp cracks; this enables derefinement of the refined elements. Crack-tip subdomains move as cracks propagate in a fully automatic process. The continuity of the displacement field in the interface between the phase-field refined subdomains and the XFEM region is again imposed in weak form via Nitsche's method. In this continuous-discontinuous approach, the phase-field model plays the role of a crack tracking citerion that handles in a natural manner crack branching and merging. This versatility contrasts with the limitations of classical criteria in linear elastic fracture mechanics to determine crack direction (e.g. maximal tensile stress criterion, stress intensity factor criterion).

The combined phase-field/XFEM approach [3] is tested with the same set of examples as the plain phase-field approach [2]. A very good agreement is obtained in terms of force-displacement response and crack path, with a signicant decrease in the computational cost: whereas the number of degrees-of-freedom in the phase-field approach increases as the cracks propagate and more elements are refined, it stays essentially constant in the combined approach, because refined elements are only needed in the crack-tip subdomains.

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Investigation of crack propagation in multi-layered media using an adaptively refined phase-field approach

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Fracture propagation in layered subsurface media is actively studied by engineers, and geoscientists. In various geo-engineered systems, such as, unconventional hydrocarbon reservoirs, enhanced geothermal systems, tunnels, and mines, fracture patterns in the subsurface play a critical role. Predictive numerical simulations are an essential tool to facilitate well-designed subsurface systems. However, despite significant advances in recent years, numerically predicting fracture propagation in the subsurface remains an outstanding challenge for the computational mechanics community [1]. This is partly because the subsurface is highly heterogeneous and contains several layers with distinct mechanical properties. The presence of these heterogeneities significantly affects the propagation of fractures in the subsurface. Depending on prevailing conditions of contrasts in elastic moduli, fracture toughness, layer thickness and in-situ stress of surrounding layers, cracks may either arrest, penetrate, or branch at the material interface [2]. Furthermore, the interface strength also plays a crucial role in the eventual crack topology in the subsurface.

In this study, we used an adaptively refined phase-field framework of Muixì et al. [3], originally developed for homogeneous materials, to investigate various failure mechanisms in layered materials. Firstly, we simulated three layered models without pre-existing flaws and with mismatch in mechanical properties (such as elastic stiffness mismatch and fracture toughness mismatch) under tensile loading. Through these models, we study the effect of heterogeneous mechanical properties on the competition between crack penetration and branching at the layer interface. Secondly, we vary the thickness of the sandwiched layer to examine its effect on the crack patterns in the middle layer. Thirdly, we studied the combined effect of confining pressure and material mismatch on crack nucleation and delamination along the layer interface. Finally, we examine the effect of weak interfaces on crack deflection and penetration at layer boundaries. We incorporate interface weakening in our model by adding interface energy term to the bulk elastic and fracture energy contributions following Kuhn and Muller [4]. The outcomes of this numerical study provide valuable insight into the various failure mechanism in multi-layered systems.

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Phase-field damage models for time-discontinuous crack evolution

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The modelling of damage behaviour has been an intensively researched topic for decades – both from the mechanical as well as from the mathematics point of view. Since the modelling of sharp cracks/interfaces and the resulting free boundary problem has been shown to be numerically very challenging, phase-field theories have become very popular, cf. [1].

Within this talk, the focus is on rate-independent damage models and their implementation. In this case, the resulting phase-field approximation is characterized by (incrementally defined) non-convex optimization problems. This non-convexity leads to two problems addressed here:
1. A discontinuous evolution of the crack in time (so-called brutal crack growth) might occur. Therefore two different internal time-scales have to be considered and modeled.
2. Different mathematical solution concepts are applicable to these kinds of rate-independent systems which are generally not equivalent, for instance the concepts of global energetic solutions and balanced viscosity solutions are here to be named. In combination with a time-discrete numerical approximation it is necessary to prove the convergence to one of the solutions concepts, see [2]. Furthermore these approximations have to be carefully evaluated with respect to the predicted physics.

One mathematically sound concept bridging the different, aforementioned time-scales is the time-discrete scheme proposed by Efendiev & Mielke, cf. [3]. Within this talk, the framework [3] is implemented into the Finite-Element-Method and carefully analysed from a physics point of view, see [4]. Particularly, the implementation and effect of the different norms and time-increments in the framework [4] are investigated by the means of numerical experiments.

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An Extended Phase-Field Method (XPFM) for 3D Fracture Simulations

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The simulation of cracks and their initiation, propagation, branching and coalescence can be an important assistance to evaluate real structures and assess their robustness and resilience. However, for this the application to 3D may be necessary. Especially for more challenging cracking processes like branching and coalescence, this poses a difficulty, since complex crack geometries can occur. This makes the discrete representation of cracks in three dimensions highly complicated.

To remedy this, a smeared approach to cracking can be helpful, like within the phase-field method (PFM) [1]. Here, the crack is reproduced with the help of a scalar field, the phase-field, indicating the crack. Its propagation is calculated using an energy approach, preventing the need for additional crack propagation criteria. One drawback, however, is the high computational effort necessary to be able to approximate the phase-field, the displacement field and their respective gradients sufficiently accurate, which is amplified vastly in 3D.

With the presented extended phase-field method (XPFM) [2] this difficulty is overcome due to an ansatz transformation of the phase-field. Embedding a standard polynomial ansatz into an exponential function enables an improved approximation of the phase-field even if rather coarse meshes are employed. Still, the crack is allowed to develop freely with no restrictions with regard to the mesh geometry. The degrees of freedom themselves attain a level set type quality. This is useful when it comes to the displacement approximation, which requires special attention due to its high gradient across the crack. Here, similar to the extended finite element method (XFEM) [3], the displacement ansatz is enriched by a function, containing properties of the expected solution. Since the enrichment function is directly coupled to the phase-field ansatz, the steep slope across the crack can be reproduced, even without a discrete approximation of the crack.

Special attention is given to the integration method. The standard Gaussian approach is not sufficient here, due to the exponential ansatz space of the phase-field on one hand and due to the non-polynomial enrichment function of the displacement field on the other hand. Additionally, the location of the crack within the finite element is generally not known a priori. In 2D, an adaptive approach based on the even subdivision of the triangular elements is chosen. However, the adaptation to 3D of this scheme is not straightforward, since the subdivision of tetrahedral elements does not yield even-sized subtetrahedra. With iterative refinement, the subelements grow evermore distorted and the integration scheme becomes less efficient as a consequence. Therefore, an adjusted approach to the subdivision of the tetrahedra has to be taken [4].

The XPFM combines the advantages of the classical PFM and the XFEM and is therefore able to reduce the necessary number of degrees of freedom significantly in comparison to other methods while still producing accurate results. This is shown by its application to several examples for simulating fracture in 3D.

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Regularised Fracture Models Based on Representative Crack Elements

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The energetic description of a crack dates back to GRIFFITH, who has related the required energy to create a crack increment to the available potential energy in the system. A variational formulation of the crack problem

$$\mathcal{E}(\boldsymbol{u}, \mathcal{B}^\Gamma) = \int\limits_{\mathcal{B}\setminus\mathcal{B}^\Gamma} \psi(\nabla \boldsymbol{u})\, \mathrm{d}V + \int\limits_{\mathcal{B}^\Gamma} \phi(\llbracket \boldsymbol{u} \rrbracket)\, \mathrm{d}A \rightarrow \min_{\boldsymbol{u}, \mathcal{B}^\Gamma}$$

is known as *free discontinuity problem*, where the size and location of the crack domain $\mathcal{B}^\Gamma$ is unknown. Two regularisations for this problem are under strong developed and are applied to brittle fracture, namely phase-field fracture [1] and eigenfracture [2].

The prediction of the crack state (opened/closed) and the forces, which can be transferred through a crack, are essential for the post-fracture behaviour but also for the calculation of the potential energy available to drive the crack. The authors have proposed to determine the deformation kinematics of a crack from discrete crack models and to couple them to the regularised fracture model by means of computational homogenisation. We have derived efficient numerical solution schemes for these *Representative Crack Models* in the context of phase-field fracture [3] and eigenfracture [4] among others. The obtained formulation is consistent to the spatial derivative, which was shown for free discontinuity problems at the discontinuities [5] and is covered by the Γ-convergence proof in [2] for linear elastic fracture problems.

In this talk, we present applications of the framework to material and geometrical nonlinearities, e.g. visco-elasticity [6], anisotropic plasticity, crack surface friction and finite deformations, as well as applications to multi-physical material models, like thermo-mechanics with heat radiation through the crack [7] and electro-mechanics with different permeability models for the crack gap [8].

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A Numerical Framework to Analyze the Conductivity of 3D Printed Tracks under Mechanical Loading.

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In recent years, the production of lightweight and complex structural parts with embedded electronics and fully encapsulated interconnecting conductive tracks has evolved due to the application of additive manufacturing techniques. Conductive ink formulations with functional nanomaterials are printed using direct writing techniques to create the conductive connections between the electrical components in electronic products [1-2]. The electro-mechanical performance of these printed tracks, typically characterized through their effective resistivity under mechanical loading, strongly depends on the composition of the conductive inks and the microstructure obtained after processing of these inks.

To analyze this functional performance, a framework is presented for the electromechanical analysis of conductive materials that provides insight into the influence of mechanical strains on the formation of cracks and the subsequent increase of resistance in conductive materials. In the proposed multi-physics model, the behavior of the conductive material is described in terms of its mechanical- and electrical response, and an auxiliary crack phase-field variable that accounts for damage development and crack propagation. The phase-field approach to brittle fracture is adopted to model the crack propagation in a diffuse manner as proposed in numerous studies [3-4] before. Existing models are altered and extended for the application to conducting media and the electro-mechanical failure analysis of these materials.

It is assumed that the increase in effective resistivity is a direct consequence of damage, i.e. fracture of the solid microstructure of the conductive medium, which is exclusively caused by the mechanical strains imposed on the body. The accumulated damage then results in direct degradation of the mechanical stiffness and the electric conductivity as a consequence of the increasing mechanical crack openings.

As an input for the model, representative volume elements of the complex microstructure are generated either based on experimental data, from FIB-SEM images & CT scans, or syntactically created based on ink characteristics and process conditions of the printed material.

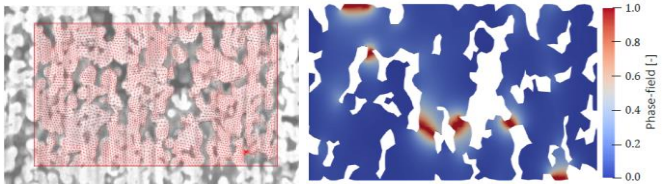

Figure: Left: Geometrical representative example of a porous layer of a 3D printed conductive material. Right: Phase field after loading.

The effective resistivity under mechanical loading is quantified as a representative measure for these conductive tracks. An increase in resistivity is observed, which is caused by crack formation in the track, which is consistent with the trends observed in experiments.

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Experimental characterization and numerical modeling of a DCDC test for a thermoplastic polymer

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Joints for wind turbine blades are mostly cross-linked polymers such as epoxy that cannot be recycled. This work aims to validate the mechanical strength of a new range of thermoplastic acrylic joints of the same chemical nature as the polymer matrix of wind turbine blades. The use of thermoplastic will increase the recycling of materials for this application.

We are interested here in the study of bulk thermoplastic polymer, at a glassy state for room temperature. Characterization of the mode I cracking of the polymer is performed using a hole parallelepiped sample under compressive load to which two initial pre-cracks at the poles of the hole were added in alignment with the compression loading (DCDC test) [1]. The energy restitution rate G_c is estimated using two analyses. The first one corresponds to classical finite element calculations in a linear elasticity framework, considering the initial structure with different crack lengths. However, the results depend on the speed of solicitation. Therefore, a second method will use finite element simulations including a phase field approach which is based on the regularization of the variational formulation of fracture [2]. This modeling approach has been shown to work remarkably well in tension, but its interest for fracture under global compressive load is still under question. To model the DCDC test, this numerical method will be used in the linear elasticity framework and fragile fracture. It will then be extended to the visco-plasticity case (perfect plasticity and hardening) to model ductile fracture and introduce plastic dissipation as proposed by Alessi and al. [3].

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Fracture in viscoelasticity: Comparison of a phase-field and a lip-field approach

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The present work provides a comparison of one particular phase-field damage model and a lip-field damage model for viscoelastic fracture.

Fracture in viscoelasticity is a complex phenomenon due to a) its highly rate-sensitive behavior b) a significant amount of viscous dissipation happening in the bulk of the material around the crack tip c) added fracture toughness due to inertial effects for rapid crack growth. In this context, we are interested in the quasi-static response of a viscoelastic material subjected to damage. An incremental variational formalism has been proposed which allows embedding the local constitutive equations into a global incremental potential. The local constitutive equations to describe the viscoelastic behavior are represented using the Generalized Kelvin Voigt (GKV) model. The minimization of the global incremental potential with respect to the state variables then gives the solution to the mechanical problem. The definition of this incremental potential is such that only free energy contributes to damage growth.

The potentials considered for both phase-field [1], [2] and lip-field [3], [4] models are quite similar locally. Damage models in the local sense are well known to introduce spurious mesh-dependent results due to the loss of ellipticity of the mathematical problem. Introducing length scales into the model is the common way to circumvent this issue. The length scale in the phase-field model is introduced by the addition of a gradient term in the potential. In contrast, the lip-field preserves the potential in local form and the introduction of length scale is through the addition of a new space called Lipschitz space and constraining the lip-damage field to lie in this space.

The potentials considered for phase-field and lip-field models are convex with respect to each state variable separately. Moreover, the admissible spaces for the state variables are also convex. Hence an alternating minimization is used to solve for state variables at each time step until convergence. In contrast to phase-field, the minimization to find the lip-damage field is greatly simplified by the use of local/non-local minimization split [4]. This allows performing the expensive non-local minimization only in the region where the damage gradient is higher than the admissible value.

The length scales of both models are selected to have similar damage profiles. The model parameters are also calibrated to obtain the same surface fracture energy. Numerical results are then provided for the bi-dimensional tests. Both models are able to capture the rate-dependent effects typically observed in viscoelastic fracture. Moreover, qualitatively similar results are observed for both models. However, the phase field model is found to be more dissipative in nature.

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Phase-Field Modelling and Computation of Fracture in Multiphase Materials

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Polycrystalline materials are widely used in engineering and material science applications, e.g. automobile, aerospace or renewable energy. The actual microstructure of the material at meso- and microscopic scales has a tremendous effect on the mechanical properties of the material and especially on the fracture toughness. Since fracture is the major failure mechanism in most construction materials, it is vital to analyze and to understand the fracture performance of polycrystals at the meso- and microscopic level. There are two main types of fracture observed in failed polycrystalline materials: intergranular and transgranular. The intergranular fracture follows the grain structure where the cracks mainly propagate along the grain boundaries. Transgranular fracture is associated with the cracks which mainly go through the grains interior. The competition between intergranular and transgranular cracking depends on the relation between the grain boundary energy (excess of energy at the boundary between two grains compared to the bulk energy of the grains) and the free surface energy (excess of energy of the free surface compared to the bulk energy of the grains). The studies in the literature have shown that the crack path strongly depends on local differences in toughness (grain interior versus grain boundaries), which significantly influences the macroscopic response of the entire structure. Hence, understanding microstructural effects in polycrystals is crucial to predict the damage mechanisms and requires considering a full complexity of the phenomena in mesoscale. In general, conventional methods (such as the extended finite element method (XFEM), cohesive zone models (CZM) or Linear elastic fracture mechanics (LEFM)) cannot capture all details of the defects in polycrystals (such as inter- and transgranular fracture) which is a major challenging task to study.

Nowadays, the phase-field method has established as one of the promising tools for the description of crack propagation in different kinds of materials. While phase-field approaches to describe crack evolution in solids are well-developed [1, 2], generalization to fracture in polycrystalline materials is still a challenging task. In particular, the multiphase-field theory is a perfect tool to study the crack propagation in polycrystalline media, because the interface energy between any pair of grains and surface energy are the natural input parameters for the model [3].

The main purpose of this study is to develop a comprehensive multiphase-field model for fracture in a multiphase system. Theoretical analysis is complemented with developments in computational modeling of the fracture phenomena. The model is implemented inside the open source software project OpenPhase to solve some examples in three-dimensions. The model reproduces well different cases. It is shown that how the competition between intergranular and transgranular cracking depends on the relation between the grain boundary energy and the free surface energy.

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Isotropic and anisotropic Eikonal gradient-enhanced damage models: thermodynamics derivation and simulation of quasi-brittle materials

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Quasi-brittle materials are often modeled using strain-softening continuum damage models. This implies using the so-called regularization techniques to obtain mesh-independent results in a finite element context. Non-local models of integral [1] and gradient [2] type, introduce an internal length in the analysis and may recover mesh objectivity in terms of structural response but are not capable of reproducing realistic "pseudo-crack" paths. In these approaches, non-local interactions are assumed isotropic and constant. This induces some drawbacks, such as boundary effects and damage spreading, leading to nonphysical damage evolution and propagation.

The Eikonal approach [3] considers that the damage field is responsible for modifying the interactions. A damage-dependent Riemannian metric is introduced in the formulation, such as damage is considered to curve the space where the interactions occur. Material points separated by damaged zone thus progressively reduce their interactions and no longer interact for very high damage levels. Consequently, the behavior becomes local, allowing for a better modeling of strain localization and the progressive transition from diffuse micro-cracking to fracture [4, 5].

The present contribution first provides a thermodynamics derivation of a gradient-enhanced Eikonal damage model (ENLG). Contrary to the usual developments for non-local models, this paper derives the problem from the micromorphic framework proposed in [6]. A purely geometric (using differential geometry concepts) modification of the free-energy potential introduced by [7] for the classic implicit gradient model is proposed. Both isotropic and anisotropic ENLG damage models are derived.

Then, numerical simulations of a few well-known problems (four point bending, shear band, etc.) using the ENLG model and a standard implicit gradient formulation are illustrated to highlight advantages and drawbacks of considering damage-dependent non-local interactions.

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"Lip-field" regularization of anisotropic damage

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Continuum Damage Mechanics aims to describe the continuous degradation of the mechanical properties of materials. Softening stress-strain responses, however, lead to strain and damage localization. From a mathematical viewpoint, this induces a loss of uniqueness in the solution of the rate equilibrium problem to be solved. From a numerical perspective, this translates into a pathological dependency of the structural response on the discretization of the spatial domain. Nonlocal enhancements and regularization techniques are used to make the response independent of the finite element mesh.

The recently proposed "Lip-field" approach [1, 2] belongs to the second class of techniques. According to this approach, the unknown displacement and damage fields are computed via the alternated minimization of an incremental potential over each time step. Contrary to what is done in phase-field models, in the "Lip-field" approach, only the so-called local potential is minimized, and a Lipschitz continuity constraint introduces damage regularization on the damage field. This ensures the boundedness of the damage gradient over the domain and naturally introduces an internal length parameter.

While this approach is attractive due to its sound mathematical framework, it seemed limited to isotropic damage formulations. However, damage-induced anisotropy should be considered when modeling certain materials (e.g., quasi-brittle materials such as concrete).

In the Continuum Damage Mechanics framework, this can be done by using a tensorial damage variable (see *e.g.*, [3]). The tensorial nature of these models makes it more challenging to use certain regularization techniques. In particular, the question of their suitability for variational-based regularizations is left open.

The present contribution proposes the first "Lip-field" formulation for anisotropic damage. A variational formulation of anisotropic damage is developed. To describe the induced anisotropic material behavior, we define a convex free-energy potential according to [3]. This model is numerically attractive due to the unboundedness of its tensorial damage variable (the so-called Ladeveze damage tensor). The model's definition of a potential guiding dissipation is a crucial aspect. This choice is directly related to the definition of a proper scalar variable on which the Lipschitz-continuity is imposed. In this formulation, we introduce a so-called "accumulated damage" variable. This allows rewriting the potential to be minimized with regards to this scalar variable while the anisotropic nature of damage growth is taken into account via the evolution law. Thus, the minimization can be naturally performed on this variable, and by enforcing its Lipschitz-continuity, one can effectively prevent localization while keeping the anisotropic properties of the model.

The proposed model is implemented in a finite element code to demonstrate its feasibility and advantages over a purely isotropic approach.

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Deterministic and stochastic phase-field modeling of anisotropic brittle fracture

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Anisotropic materials with cubic lattice such as silicon exhibit a four-fold symmetry in their elastic as well as fracture properties. Such materials are characterized by two weak directions that are equally favourable for crack propagation. In certain orientations of the material, the two weak directions are located symmetrically with respect to the loading. This leads to the distinctive phenomenon of the crack alternating between the two weak directions as it propagates, resulting in saw-tooth or zigzag crack patterns.

In this work, we investigate the variational fourth-order phase-field formulation of anisotropic brittle fracture to model crack zigzagging. We analytically derive and numerically test the fundamental behavioral aspects predicted by the two main available models [1, 2]. In this regard, the presence of second gradients of the phase-field variable in the weak form demands C_1 continuity of the shape functions for finite element discretization. To this end, we adopt isogeometric analysis [3] and discretize the displacement field, the phase-field and, as per the isoparametric concept, the geometry by quadratic B-Splines.

Furthermore, non-uniqueness of the phase-field solution associated to non-convexity of the governing energy functional [4] is observed to be quite pronounced in the anisotropic case (more than in the isotropic case). Hence, we transition from a deterministic to a stochastic model by introducing a material-related random field in the anisotropic phase-field energy functional. We introduce a small perturbation to the direction-dependent fracture toughness to trigger multiple crack-paths. We employ Monte Carlo, randomized quasi-Monte Carlo sampling and surrogate-based approaches to estimate statistical moments of the phase-field variable.

Numerical results establish the large variation in the responses of the two fourth-order phase-field models, both in their deterministic and stochastic versions. For either modeling choice, the stochastic model, which captures several possible zigzag crack paths, holds significant promise to enable meaningful predictions of anisotropic fracture with phase-field models.

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Assessment of a phase-field model with orthotropy-based energy decomposition to predict mixed-mode fracture in rocks

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In geomechanical applications, determining the fracture growth trajectories in rock formations under complex stress regimes can be challenging, particularly when the rock is anisotropic. Mixed-mode loading and rock anisotropy interact with each other to determine the fracture growth trajectory [1]. This interaction can either strengthen or weaken the individual effects as shown in many studies (e.g. see [1, 2]). To address this complexity, this study employs the phase-field model proposed by [3], in which the strain energy density is decomposed based on the generalized Miehe decomposition for orthotropic materials. The model is used to predict the fracture trajectories in transversely isotropic rocks under fixed mixed-mode loading ratio.

To maintain a constant mode mixity, an asymmetrical semi-circular bend test is used. This test setup was proposed by [4] and has been used in [5] for pure mode I tests. The sample geometry remains constant for different sets of tests, each with a fixed mode mixity, while the orientation of the isotropy plane (i.e. the foliation plane in the Grimsel Granite) with respect to the main notch varies. Here we consider the results from 99 fracture toughness tests on metamorphic Grimsel Granite under four different ratios of mixed-mode I/II loading.

The performance of the phase-field model is assessed by comparing the results from the simulations with those obtained from the experiments. The comparison focuses on the fracture load, fracture initiation angle, and fracture path. To assess the robustness of the method, we compare the sensitivity of the kink angle predictions to the mesh size and the length of fracture process zone between the phase-field simulations and those performed in [6] with the extended finite element method.

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Interactions of Phase Transformation and Crack Propagation in Anisotropic Microstructures

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The world's escalating energy demand for cooling has triggered the development of advanced materials and technology for energy conversion, with special consideration for the mitigation of greenhouse gas emissions. Recent research in this field has been concentrated on solid-state refrigeration utilizing the elasto, electro, or magnetocaloric effect, which is governed by a displacive and diffusionless mechanism known as martensitic phase transformation (MPT). MPT between the parent phase (austenite) and the product phase (martensite), commonly observed in various steels, shape memory alloys (SMAs), and ceramics, is accompanied by formation and evolution of microstructure. When it comes to design and application of these materials in multiphysics environments, a crucial attention should be paid to interactions between fracture and MPT, which are a highly important problem in the material science and engineering.

In this work, a coupled problem of crack initiation and propagation and two-variant MPT in anisotropic microstuctures is developed based on a phase field approach [1]. The model established includes a coupled system of three time-dependent Ginzburg-Landau (TDGL) equations [2], which describes the evolution of damage variable, two martensite variants, and the quasi-static equilibrium equation, respectively. Therefore, it is able to characterize evolution of the distribution of austenite and two martensitic variants as well as crack growth in terms of corresponding order parameters. This work accounts for the positive dilatational component of the transformation strain, which accompanies the MPT from austenite to martensite phase, leads to an eigenstrain within the martensitic phase. Since the eigenstrain resultsin both tensile and compressive parts, the model considers the sign of the dilatational component. The model is established based on a coupled system of the TDGL equations and the equilibrium elasticity equation, and it explains the evolution of distributions of austenite and different martensitic variants in terms of corresponding order parameters. To this end, two-variant martensitic microstructure consists of austenite and two martensitic variants and is represented in terms of the distribution of two order parameters. Transformation strain transforms crystal lattice of austenite into crystal lattice of martensitic variant. In addition, a constraint for the order parameters describing transformation strain is imposed. This can be done by constructing a Landau-type polynomial energy function to characterize the transformation among different martensitic variants.

The results obtained show the crack propagation does not start until MPT has grown through the microstructure to some extent. Moreover, load-displacement curve of microstructure specimen with isotropic and anisotropic elastic constants with different crystal lattice orientation have been discussed. Last but not least, two polycrystalline models have been built to study the coupled approach of fracture and phase transformation in polycrystalline microstructures.

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Fatigue crack propagation with a phase-field approach coupled to adaptive mesh refinement and cycle jump schemes

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In recent years, the phase field approach applied to crack propagation problems has gained in popularity in the scientific community. So much so that even if it was originally applied to brittle fracture (e.g. Ref. [1]), it was since extended to several other crack propagation mechanisms such as fatigue in Ref. [2]. This popularity can be explained by the flexibility of the phase field model in a finite element framework in the context of crack propagation. Indeed, it has been shown to recover complex crack patterns without adding additional propagation criterions. However, these models usually suffer from prohibitive computing time. Such efficiency issues makes it difficult to study application of industrial cases, or to perform numerical-experimental comparisons. Consequently, in this work we put forward the coupling of multiple tools to accelerate computing time of phase field fatigue crack propagation simulations. First, an adaptive mesh refinement procedure (AMR) is implemented to optimize the number of degree of freedom processed at each time step. Then an iterative cycle jump scheme inspired by Ref. [3] is coupled to adaptive mesh refinement to optimize the number of computed cycle.

It is indeed well known that using a phase field model in a finite element framework suffers from multiple efficiency drawbacks. Firstly, the regularisation of the crack discontinuity on a small length scale means that in order to capture the gradients of the physical quantities in the damage zone, a very fine mesh must be used. Since for most crack propagation simulations, crack path is not known a priori, the whole structure must be meshed very finely, yielding very high computing time. Conversely, by coupling AMR and phase field, we can use a refined mesh only where it is necessary, yielding faster computation while keeping precision. In this work a refinement criterion based on the value of the phase field is used to achieve a flexible coupling between phase field and AMR.

Secondly, the computation of a single cycle can lead to a high computing cost because of the high nonlinearity of the damaged structure behaviour. Moreover, in the case of high cycle fatigue lifetime prediction, lifetime typically consists of $N > 10^5$ cycles. In this context, we use an implicit cycle jump scheme coupled to the previously introduced fatigue phase field AMR. This iterative approach enables us to skip large number of cycles while keeping a predefined precision.

To demonstrate the capabilities of the model, multiple benchmarks of the phase field fracture literature are first studied. We validate that the introduced AMR and cycle jump schemes yield precise and efficient results and couple them both to achieve maximum efficiency gains. First, several cases of mode I crack propagation are studied to validate the coupling. Then we demonstrate the ability of the model to recover more complex crack propagation patterns such as crack kinking, branching, nucleation and coalescence.

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High temperature fatigue crack growth modeling in Ni-based superalloys using a gradient-enhanced elastic-viscoplastic damage model

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Fatigue crack growth prediction during both design and lifespan analysis of aeronautical structures still remains of great interest to ensure safety and reliability of critical components. Disregarding the conventional concepts from the Linear Elastic Fracture Mechanics (LEFM) theory, this study focuses on a new approach to evaluate the fatigue crack propagation in Nickel-based superalloys. It consists in assessing the capabilities associated with the local approach to fracture to simulate the propagation of a long fatigue crack in structural components [1]. To this end, a three-step approach is considered.

First, the cyclic non-linear behavior of the recently developed Nickel-based superalloy AD730™ is studied using dedicated characterization tests at three target temperatures (20, 550 and 700°C). The main strain-hardening mechanisms as well as complex viscosity effects are evidenced. A set of constitutive equations for the cyclic non-linear behavior of AD730™ is proposed and calibrated following the pioneer work of [2]. A good agreement between experimental and simulated results is achieved.

Next, high temperature fatigue and dwell-fatigue crack propagation tests on SEN-T specimens are performed in order to evidence the main crack driving mechanisms. A strong behavior-damage coupling is then settled – using the Continuum Damage Mechanics (CDM) concepts – hence leading to a time-incremental damage model for fatigue [3]. This model is implemented in a finite element code using a fully implicit resolution scheme. In order to solve for the spurious mesh-dependency effect, a non-local extension of the damage model is proposed using an implicit gradient formulation [4]. Several numerical tests of increasing complexity illustrate the ability of this non-local formulation to efficiently control damage localization and subsequently to ensure convergence of the numerical results upon mesh refinement.

Finally, an error-based mesh adaption procedure is considered in order to refine the mesh in the fracture process zone, close to the crack-tip where the non-linear phenomena occur. Once crack onset is achieved, a crack path tracking algorithm is used to evaluate the geometry and the direction of the crack increment [5]. Then, a damage-to-crack transition consisting in remeshing steps, fields transfer and equilibrium recovery is performed. This way, crack growth kinetics can be captured. The whole numerical loop is assessed on calculations conducted on a SEN-T specimen subjected to complex fatigue and creep-fatigue loading conditions. The capabilities of the proposed approach to relate the results from CDM to those from LEFM are emphasized, while its limitations are also discussed.

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An eXtended Phase-Field Method (XPFM) for the Simulation of Fatigue Fracture Processes

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Most engineering structures undergo changing cyclic loads which can lead to fatigue fracture and failure. Nowadays, numerical methods can help to facilitate an estimation of the life span of these structures. Among others, the eXtended Finite Element Method (XFEM) [1] and the Phase-Field Method (PFM) [2] are methods which can deal with crack propagation processes. During the last decade, the PFM gained increasing popularity because crack phenomena like crack initiation, propagation, branching and merging can be handled without the need for further criteria like within the XFEM. The effort of implementation is also lower compared to the XFEM, but the computational costs are quite high since a rather fine finite element discretisation around the crack is necessary in order to achieve an acceptable low error. Nevertheless, a mesh-independent crack representation is, contrary to the XFEM, not possible. Without loss of accuracy much coarser meshes can be applied in the XFEM compared to the PFM.

Recently LOEHNERT ET AL. [3] proposed the eXtended Phase-Field Method (XPFM). This method combines benefits of both, the XFEM and the PFM. A transformed ansatz for the phase-field is introduced, based on the exponential solution of the one-dimensional phase-field problem in [2]. Furthermore, an enriched displacement field ansatz, where the enrichment functions are coupled to the transformed phase-field degrees of freedoms, is added. Herby it is possible to retain the crack initiation and propagation characteristics of the underlying phase-field approach on much coarser meshes independent on the orientation of the finite elements. Thus, the number of degrees of freedom can be reduced significantly in contrast to the original phase-field approach.

A phase-field model for fatigue fracture processes has been presented by CARRARA ET AL. [4]. There, a history-depended degradation of the fracture toughness is proposed. The model is able to reproduce fatigue phenomena like WÖHLER curves or the PARIS law. In this contribution, this fatigue approach is coupled with the developed XPFM for the two-dimensional case. It is shown, that the features of the phase-field fatigue model can be reproduced despite the reduced numerical effort of the XPFM on coarser meshes.

Due to the non-linear transformed phase-field ansatz and the non-polynomial enrichment functions, a sufficiently accurate integration method is required apart from standard GAUSS-integration. Beyond, an adequate convergence criterion for the nested staggered and enrichment update solution process is discussed. Several numerical examples are shown to demonstrate the coupled extended phase-field fatigue method.

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A phase-field model describing Paris' fatigue law

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Fatigue is one of the most critical and less predictable phenomena in nature, affecting the mechanical behavior of materials. Engineers currently use the Griffith's fracture law to assess the structural limits under monotonically increasing loads and Paris' law to estimate the structural life under cyclic loads. These two fundamental laws governing the failure of structures in the short and long run have often been seen as disconnected in the scientific literature. The first formal link between the two fields was established in some seminal, but somewhat unknown, papers by Marigo and coworkers; see [1, 2, 3] and citations therein. In [1], the authors present a detailed derivation of this link and its fundamental ingredients: in the case of a peeling test, it is shown how a sequence of cohesive fracturing processes due to cyclic loading at the micro time scale can accumulate to form a steady-state propagation at the macroscopic time scale. The prefixes micro and macro for the time scales are related to the small parameter d/L measuring the size of the cohesive zone with respect to the size of the structure. An implicit law is derived connecting the macroscopic time rate of the crack length to the ratio G/G_c between the actual energy release rate G and the material toughness G_c. The very same law reduces to Paris' fatigue law when G is much smaller than G_c, while it tends to the Griffith's law when G approaches G_c from below.

From these results [1, 2, 3], we have deduced a phase-field model having this dual capability of describing both sudden and accumulated fracture phenomena. The approach is based on the least energy principle where the total energy of the structure, to be minimized, is the sum of the elastic energy and a dissipation potential, taken as a power function of the newly created crack surface. Then, we implemented the model via FEniCSx [4], observing promising results: in a pre-notched rectangular sample with mode I cyclic loading conditions was possible to retrieve standard pre-assigned path cracks. The code was also tested in a less trivial case considering, instead, a mixed I-II mode solicitation, where we observed the initiation of the crack and its subsequent complex path propagation.

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Minisymposium TF:

Theory of fracture, crack propagation criteria and crack tracking algorithms

Organized by M. Ortiz and A. Pandolfi

Dynamic crack growth in viscoelastic materials with memory

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We study a model of crack growth in viscoelastic materials based on the following ideas (see [4]):

(a) the displacement solves viscoelastodynamics out of the crack, with traction-free boundary conditions on the crack;

(b) the dynamic energy-dissipation balance is satisfied: the sum of the kinetic energy and of the elastic energy at time t, plus the energy dissipated by viscosity and crack growth between time 0 and time t, is equal to the initial energy plus the total work done by external forces between time 0 and time t;

(c) a maximal dissipation condition is satisfied, which forces the crack to run as fast as possible, consistent with the energy-dissipation balance.

It is known (see [3]) that in the Kelvin-Voigt model of viscoelasticity conditions (a) and (b) prevent crack growth (viscoelastic paradox). To overcome this problem we study a different viscoelastic model, the Maxwell model (see [5]). It is governed by the following system, containing a memory term:

$$\ddot{u}(t) - \operatorname{div}\big((\mathbf{C}+\mathbf{V})Eu(t)\big) + \operatorname{div}\Big(\int_0^t \mathrm{e}^{\tau-t}\,\mathbf{V}Eu(\tau)\,\mathrm{d}\tau\Big) = \ell(t),$$

where $u(t)$, $Eu(t)$, and $\ddot{u}(t)$ are the displacement at time t, the symmetric part of its gradient, and its second derivative with respect to time, $\mathbf{C}$ and $\mathbf{V}$ are the elasticity and viscosity tensors, $\ell(t)$ is the external load at time t, and the system is satisfied out of the crack.

We prove an existence result in the case of planar elasticity with a free crack path, with suitable a priori assumptions on the regularity of the crack and of its time evolution. Also the maximal dissipation condition is satisfied only among suitably regular competitor cracks.

The proof is based on a careful analysis of the properties of the solution of the system with given initial and boundary conditions, in the case of a prescribed time dependent crack. In particular, to prove the result with a free crack path (see [1]) we use the results on existence, uniqueness, and continuous dependence on the cracks obtained in the case of prescribed time dependent cracks (see [2] and [6]).

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Optimal scaling laws for ductile fracture derived from strain-gradient microplasticity

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Ductile fracture is the process whereby a material separates across a failure surface through mechanisms, such as void nucleation, growth and coalescence, that entail large amounts of plastic work. Such extensive plastic deformation notwithstanding, ductile fracture remains quintessentially a fracture process, in the sense that failure takes place by separation across a plane or surface and entails a well-characterized amount of energy *per unit area*, or *specific fracture energy*, to operate. Experimentally, ductile fracture is easily identified fractographically, as the crack surfaces exhibit a characteristic dimpling—the dimples being vestiges of voids—that is in contrast to the sharp specular cracks that result from brittle fracture. Furthermore, the measured specific fracture energies attendant to ductile fracture, e. g., from Charpy tests or from J-testing, are much larger than those of brittle solids.

We [1, 2, 3] carry out an optimal-scaling analysis of ductile fracture in metals. We specifically consider the deformation, ultimately leading to fracture, of a slab of finite thickness subject to monotonically-increasing normal opening displacements on its surfaces. We posit two competing constitutive properties, namely, *sublinear energy growth* and *strain-gradient hardening*. Sublinear growth (the energy of linear elasticity exhibits quadratic growth, by way of comparison) is a reflection of the work-hardening characteristics of conventional metallic specimens and gives rise to well-known geometric instabilities such as the necking of bars, sheet necking, strain localization and others. Strain-gradient hardening [4] has been extensively investigated and demonstrated by means of torsion tests in wires [5], nanoindentation [6], and by other means. It results in deviations from volume scaling, i. e., in *nonlocal behavior* and *size dependency*, in sufficiently small material samples. We show that ductile fracture indeed emerges as the net outcome of these two competing effects: whereas the sublinear growth of the local energy promotes localization of deformation to failure planes, strain-gradient plasticity stabilizes this process of localization in its advanced stages, thus resulting in a well-defined specific fracture energy. Specifically, we show that ductile fracture requires a well-defined energy per unit area that can be bounded above optimally by a void-sheet construction. This specific fracture energy bears a power-law relation to the prescribed opening displacement. This power-law relation may be regarded as an effective cohesive potential, thus indicating that ductile fracture is cohesive in nature. In particular, fracture processes involving distributed—possibly fractal—damage are ruled out by the analysis.

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Griffith Fracture in Viscoelastic Elastomers Done Right

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It has been long established that the Griffith criticality condition

$$-\frac{\partial \mathcal{W}}{\partial \Gamma_0} = T_c \tag{1}$$

describes the growth of cracks in elastomers subjected to quasi-static mechanical loads.

The left-hand side $-\partial \mathcal{W}/\partial \Gamma_0$ in expression (1) stands for the change in total (stored and dissipated) deformation energy $\mathcal{W}$ in the elastomer with respect to an added surface area to the pre-existing crack Γ_0 under conditions of fixed deformation of those parts of the boundary that are not traction-free.

The right-hand side T_c is the so-called critical tearing energy. It is a characteristic property of the elastomer. Importantly, it is *not* a constant. Much like $\mathcal{W}$, it is a function of the loading history. More specifically, experiments have established that T_c can be written in the general form

$$T_c = G_c(1 + f_c).$$

In this expression, G_c denotes the intrinsic fracture energy, or critical energy release rate, associated with the creation of new surface in the given elastomer. It is a material constant, independent of time. Its value is in the relatively narrow range $G_c \in [10, 100]$ N/m for all common hydrocarbon elastomers. On the other hand, f_c is a non-negative function of the loading history that scales with the viscosity of the elastomer. Precisely how f_c — and hence T_c — depends on the loading history for arbitrary loading conditions has remained an open problem for decades rendering the Griffith criticality condition in its ordinary form (1) essentially useless.

In a recent contribution, Shrimali and Lopez-Pamies [1] have uncovered a general formula for f_c — and hence T_c — and in so doing they have determined that (1) can in fact be reduced to a form that involves *not* the historically elusive critical tearing energy T_c, but only the intrinsic fracture energy G_c of the elastomer. The result hinges on the following two elementary observations.

i. For any viscoelastic elastomer, the total deformation energy $\mathcal{W}$ in (1) can be partitioned into three different contributions:

$$\mathcal{W} = \underbrace{\mathcal{W}^{\rm Eq} + \mathcal{W}^{\rm NEq}}_{\text{stored}} + \underbrace{\mathcal{W}^{v}}_{\text{dissipated}}.$$

Here, $\mathcal{W}^v$ represents the part of the total energy that is dissipated by the elastomer via viscous deformation. On the other hand, the combination $\mathcal{W}^{\rm Eq} + \mathcal{W}^{\rm NEq}$ represents the part of the total energy that is stored by the elastomer via elastic deformation. In this combination, $\mathcal{W}^{\rm NEq}$ stands for the part of the stored elastic energy that will be dissipated eventually via viscous dissipation as the elastomer reaches a state of thermodynamic equilibrium. On the contrary, $\mathcal{W}^{\rm Eq}$ denotes the part of the stored elastic energy that the elastomer will retain at thermodynamic equilibrium.

ii. "Pure-shear" fracture tests of common hydrocarbon elastomers, as well as of more modern types of elastomers, consistently show — rather remarkably — that fracture occurs from the pre-existing crack in the specimens at a critical stretch that is independent of the stretch rate at which the test is carried out.

Precisely, by combining the above two observations, Shrimali and Lopez-Pamies [1] have shown that the Griffith criticality condition (1) can be reduced to the fundamental form

$$-\frac{\partial \mathcal{W}^{\rm Eq}}{\partial \Gamma_0} = G_c. \tag{2}$$

In this presentation, I will talk about the derivation of the criticality condition (2) and its use to explain two of the most distinctive fractures tests for viscoelastic elastomers: the delayed fracture test and the trousers fracture test.

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Some remarks on a new space of generalised functions of bounded variation

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The variational approach to rate-independent evolution problems relies on a time discretization scheme, where the approximate solution at a given time is obtained by solving an incremental minimum problem which involves the solution at the previous time. In this framework, the study of crack growth in linearly elastic-perfectly plastic materials in the small strain regime leads to incremental minimization problems that involve the crack as well as the elastic and the plastic parts of the strain, which in general lack of regularity. In the generalized antiplane case the crack is represented by a rectifiable set, the elastic part of the strain is a square integrable function, while the plastic part is a measure. It is convenient to express these problems in terms of a functional which depends on the displacement. However, since the functional to be minimized does not provide a control on the jump of the displacement, there are boundary conditions for which the minimum problem does not have a solution in the space of functions with bounded variation.

In order to obtain the existence of a solution to such problems we introduced in [1] a new space of generalized functions of bounded variation. We studied the fine properties of the functions belonging to this space and proved a compactness result. We also proved the lower semicontinuity of the functionals involved in the incremental minimum problems. Moreover, by adapting a nontrivial argument introduced by Friedrich in [3], we showed that every minimizing sequence can be modified to obtain a new minimizing sequence that satisfies the hypotheses of our compactness result. Therefore the Direct Method of the Calculus of Variations can be applied providing the existence of a solution to the incremental minimum problems.

In this talk I would also like to mention some results on the Gamma convergence of related functionals recently obtained together with Gianni Dal Maso [2]. In particular, we proved that a class of integral functionals defined on this space is invariant under Gamma convergence. This result can be applied to the study of some homogenization problems, both in the periodic and in the stochastic case.

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Dynamic Versus Static Analysis of Fracture in Soft Materials

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While cracks mostly propagate dynamically, their analysis is usually quasi-static. Quasi-static analysis is simpler, of course, than the dynamic one. Will the dynamic analysis provide results similar to the quasi-static ones? We address the answer to this question in the present work. We compare results of the dynamic and quasi-static simulations of cracks initiated by quasi-static loads in aneurysm material.

We use the material-sink (MS) approach [1-4], which is based on the notion of the diffused bond breakage. The latter feature implies a local loss of material and, consequently, decrease of mass density, which, in its turn, means that both stiffness and inertia go down in the damaged zone. The cancellation of inertia is an important feature of the MS approach in contrast to more formal regularization theories as phase field, gradient damage, and other nonlocal formulations.

The MS approach is implemented within commercial finite-element software ABAQUS. A reduced mixed finite-element formulation is adopted to circumvent the volumetric locking and an implicit staggered solution algorithm is developed via the user-defined element subroutine UEL.

Considered examples show that the onset of crack instability under static loads is followed by the dynamic rather than quasi-static crack propagation. Moreover, dynamic and quasi-static simulations, generally, provide different results.

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LEFM based criterion for crack propagation under complex structural loadings

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Historically, Linear Elastic Fracture Mechanics (LEFM) based criteria rely on either stress intensity factors (SIF) or energy release rate. For 2D structures under quasi-static loading, one has to decide if the crack propagates or not and if yes in which direction. Concerning crack propagation, the classical criterion is the Griffith's criterion. It is a kind of unilateral relationship based on the positiveness of the dissipation, meaning the crack propagates if the energy release rate reaches its critical value G_c (defined as a material property) and that the energy release rate should remain at the critical value all along the failure process, the crack velocity being adjusted so that this condition is met. Concerning crack orientation, many criteria exist either based on the max hoop stress, the maximum energy, the symmetry of the loading.....In 3D, the problem is slightly more complex as the condition defined above cannot be met all along the crack front and one has to define the crack velocity profile based on SIF or energy release rate distribution along the crack front.

However, while there is a kind of consensus on the universality of this criterion and the definition of G_c, it has been shown by several authors that, even for a material like PMMA considered as a model material for brittle fracture, this criterion fails at predicting crack propagation for some specimen geometries [1, 2]. In other words, the stress field induced by structural effects (geometry, loading) and through which the crack is propagating has an influence on G_c. This is usually named 'constraint effect'. Non-local models using an smoothed description of the crack discontinuity (like phase field, non-local damage, micro-morphic damage,...) have the ability to handle this kind of situation. This is due to their internal length parameter allowing for the model to probe the material in a finite volume at the crack tip. The limitation of LEFM based criteria is thus due to their local nature, probing the material only at the crack tip through SIF. But, their much lower computational cost make them the best candidate for structural application, inducing loading for which they fail at being predictive. Elaborating *non-local* LEFM criteria is thus of huge practical importance.

Based on experimental direct estimations of SIF and higher order terms in the asymptotic expansion of the linear elastic field around the crack tip (T-stress T, B-stress B), we suggest and calibrate a stress based criterion. This criterion relies on the estimation of the stress tensor at a distance r_c of the crack tip from SIF, T and B. The two parameters of this criterion are the critical distance or internal length r_c and the critical stress σ_c. Compared to existing *generalised* LEFM criterion, our criteria is: based not only on SIF and T but it relies also on B, based on the second invariant of the stress tensor, as the usually adopted maximum tensile stress cannot account for the influence of T for pure mode I straight crack propagation, calibrated using direct experimental estimation of SIF, T, B from full-field displacement measurements (implemented in [3]) instead of using finite element models.

This formalism is convenient as the critical stress σ_c (or the fracture toughness K_{Ic}) are estimated independently on the structural effects, these effects being accounted for by the criterion itself. Based on the same idea, a generalised energy criterion can be formulated allowing for capturing even more complex situations. For validation purposes, the prediction of these criteria implemented using X-FEM is compared to the results of a validation experiment.

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Crack facet initiation in pure Mode III fracture

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Mode III, or anti-plane shear cracking, is a peculiar phenomenon. Initially, when Irwin introduced his mode decoupling theory, he assumed a horizontal crack propagation. Since then, many experiments have shown that in brittle materials, when deformed in an anti-plane manner, the original mother crack fragments into many daughter cracks with an angle different from horizontal [1]. These small facets then coalesce and continue propagating in the original direction with an increasing rugosity.

The talk focuses on the detailed analysis of the daughter crack initiation using the phase-field technique [2, 3] and the coupled criterion [4]. After our recent study on tensile and in-plane shear fracture [5], we present a comparison between the two techniques focusing on the characteristic initiation distance in pure Mode III loading conditions.

To induce instability, in the phase-field method, the critical energy release rate was varied based on a gaussian random field. We show that without any significant defect, our implementation is capable of localizing the cracks. Furthermore, we present a meticulous study of both numerical and material parameters to investigate their effect on the initiation distances.

The model was found to be very robust, and we show that only the characteristic regularization length of the phase-field model and Poisson's ratio changes the initial distance between the automatically formed daughter facets.

We extended our previous analysis [5] using finite fracture mechanics to understand the phenomenon observed in our numerical experiments. We found that the reinitiating cracks are initiated in an unstable manner but propagate stably after. This is in good correspondence with the results observed in phase-fields. Furthermore, we observed that the maximum tensile stress criterion dominates the initiation. The energy release rate in facet formation mode was significantly lower than in horizontal advancement. This results in stronger resistance. This was also found to agree with our phase-field simulations.

Interestingly, we saw that Griffith's original theory is unable to predict facet formations in pure Mode III because the existence of a finite length scale is essential. This confirms our reasoning that the addition of the regularization length scale in the phase-field fracture is crucial to capture relevant physical phenomena in crack initiation.

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Crack propagation in elastic media with anisotropic surface energy: Experiments, Phase-field simulations, Linear Elastic Fracture Mechanics

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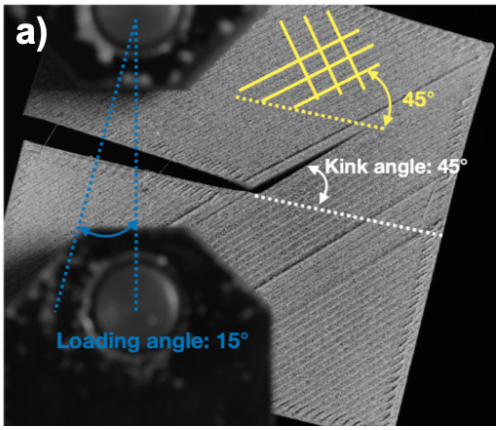
Additive manufacturing is receiving increasing attention due to its advantages in terms of modelling flexibility and allowing to easily design complex micro-structures [1]. A Recent study reports [2] achieving strongly anisotropic fracture toughness in material printed by Fused Deposition, while retaining isotropy in elasticity. The aim of this study is to explore brittle crack propagation in specimens fabricated by Fused Deposition in fracture experiments under mixed mode loading and provide numerical predictions based on a variational approach to fracture. Comparing numerical results using a strongly anisotropic phase-field model [3] with experimental data, we show the ability to predict crack trajectories and the relevant critical load for crack propagation. Such predictions can also be recovered by the generalized maximum energy release rate in a linear elastic fracture mechanics framework.



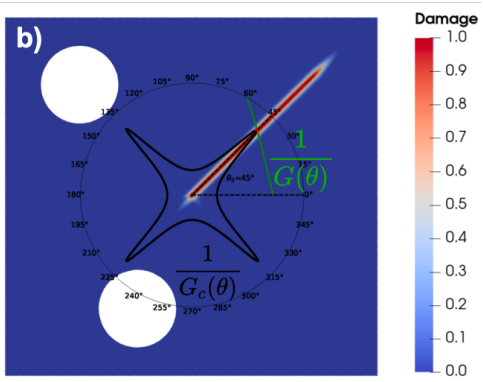


Figure 1: A kinking crack following material fibres in an anisotropic Compact Tension Shear specimen under mixed mode loading a) experimental setup and b) a snapshot of the predicted numerical crack path with 45° raster angle and 15° loading angle

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Characterising fracture behaviour of flexoelectric solids using newly proposed numerically robust mixed FE

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The size-dependent phenomenon of flexoelectricity is well-known due to its application in high-precision micro- and nano-scale MEMS. Flexoelectricity is the electromechanical coupling of strain gradients and electric field (direct flexoelectricity) or electric field gradients and mechanical strains (converse flexoelectricity). It can be observed not only in dielectrics with centrosymmetric unit cells but also in piezoelectric materials that already exhibit linear electromechanical coupling. Since flexoelectricity is associated with strain gradients that are inversely proportional to the length scale, the higher-order electromechanical coupling becomes dominant at smaller scales and often exceeds the influence of piezoelectricity. Simulation of flexoelectricity along with piezoelectricity demands fully coupled higher-order electromechanical formulations.

The fracture behavior of piezoelectric and, later on, ferroelectric materials has been intensively studied in the last decades. Recently, numerical modeling of fracture in polycrystalline ferroelectric ceramics under monotonic and cyclic electromechanical loading was performed [1]. For the numerical modeling of flexoelectricity, a second-order collocation-based mixed FEM was proposed [2] by the authors. Moreover, two new numerically robust mixed finite elements for the classical mixed FE were developed and implemented [3].

The newly proposed elements [3] are used for the fracture mechanics simulations in the current work. An edge-cracked aluminum nitride panel is modeled as a characteristic problem. The simulations go beyond conventional modeling of flexoelectricity in dielectric solids and primarily aimed at studying the mutual interaction of piezoelectricity and flexoelectricity. That is, the numerical simulations of an edge-cracked panel illustrate the influence of a higher-order electromechanical coupling contribution on piezoelectric solids.

It was found that the "smoothening" effect of strain gradient elasticity (SGE) along with flexoelectricity results in a substantial reduction of the crack tip opening displacement (CTOD). In contrast, a sudden increase followed by a smooth drop of electric potential is observed along the crack face. The inclusion of piezoelectricity in flexoelectric simulations further reduces CTOD. Furthermore, a tremendous change in the profile of the generated electric potential is observed. When the higher-order electromechanical coupling is considered along with piezoelectricity, a contradictory or superimposed behavior of the electric potential profile is observed depending on the polarity of the piezoelectric material. The dominance of the gradient terms strongly influences the results in the vicinity of the crack tip. By varying the flexoelectric coefficients, the influence of flexoelectricity on the electric potential profile along the crack surface is additionally investigated. The present work demonstrates and explores the combined action of the piezo- and flexoelectric constituents and their influence on the fundamental fracture parameters in the context of the linear elastic fracture mechanics.

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Dissection of a continuous-discontinuous strategy: a review of its elementary components

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Numerous strategies have been proposed in the litterature to obtain a discrete crack representation from a continuous model [1]. These strategies may seem rather complex and completely different if considered in their entierty. However, they can actually be decomposed into elementary components which correspond to the methods chosen to answer the three following questions:

- When to insert the discontinuity?
- Where to insert the discontinuity?
- How to resume the computation?

Such decomposition of continuous-discontinuous strategy enables to compare more easily the different procedures. Besides, these elementary components can be selected independently according to the user's requirements and then assembled together to constitue a complete continuous-discontinuous strategy.

The aim of this contribution is to provide guidelines to analyze and compare different strategies of the literature to obtain, in a post-processing step, a discrete crack representation from a diffuse damage model. The choice of the different components depends on:

- whether the variable that represents material degradation is coupled to the constitutive equations or simply a result of a post-processing calculation;
- whether the continuous model is regularized or not;
- how the discontinuity is represented;
- the necessity to capture crack branching and crack initiation away from any boundary.

In all cases, ease of implementation and computational cost are important factors in the decision process and must thus be taken into account.

In this contribution, different orientation criteria used for a local approach of fracture are considered. They lead to either a scalar field or a vector field related to the discontinuity surface. These fields serve as input data for crack path tracking algorithms that are used to obtain a continuous and regular discrete crack path. The output data then serve to define implicitely or explicitely the crack surface, with several technics enabling to switch from one definition to another. An original classification of these crack path tracking algorithms based on the input and output data nature [2] will be presented. With this approach, it is easier to see how some interesting ideas of one strategy can be applied to others. For example, the principle used for the extension from 2D to 3D crack path tracking proposed in [3] can be easily used for other 2D approaches that rely on a scalar field with a ridge. Finally, as the insertion of a discontinuity in a continuous models implies a change of discretization, different technics to transfer fields and to help retrieve equilibrium are discussed.

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Efficient prediction of 3D crack propagation using configurational forces

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In many applications, the 3D propagation of a crack is of great interest. This propagation can be predicted in FEM models either by using damage of the material or element (phase-field models), by special elements that can contain cracks (XFEM), or by discrete modeling of the crack and using classical fracture-mechanical approaches to compute the Crack-Driving Force (CDF) [1]. In CDF-based approaches, the crack is repeatedly extended by a crack increment.

The physically-based concept of Maximum Energy Release Rate (MERR) is assumed to be the most general criterion for crack propagation, which can be evaluated using trial and error by introducing a range of virtual crack extensions. The direction with the highest energy dissipation yields the crack propagation direction.

One widely used measure of the CDF is the J-integral, which has been extended using configurational forces to also be valid for non-proportional loading and inhomogeneous materials [2] and yielding a vector of the CDF. The configurational force corresponds to the gradient in potential energy for a change in geometry. It yields non-zero values at inhomogeneities such as interfaces, surfaces, and cracks. For cracks, however, this J-integral vector is only valid for a crack propagation in the same direction as the previous crack propagation direction. For a curving crack path, the configurational-force-based J-integral only approximates the crack driving force. Small crack increments are therefore needed for highly curved cracks.

By introducing a virtual crack extension and evaluating configurational forces for that crack, the accuracy of the direction to meet MERR of that virtual crack extension can be evaluated, based on the meaning of configurational forces. Therefore, the authors have developed a method that evaluates the nodal configurational forces in a FEM mesh and uses them to repeatedly correct the crack angle of the virtual crack in 2D structures [3]. This method is nearly as accurate as trial and error but much faster. Also, the method is much more accurate than directly using the J-vector for crack extension with only a slight increase in computational effort.

For 3D cracks, using trial and error an enormous computational effort is necessary to find the crack propagation direction for MERR. Such high computational effort is usually uneconomical. Therefore, in this work, the repeated crack correction concept is extended to 3D cracks and evaluated for simple cases from literature [4]. In 3D, our tool computes the direction of MERR with manageable effort for the same accuracy as trial and error. Due to the material-independent formulation of configurational forces, it is ready to be extended towards heterogeneous materials and elastic-plastic materials.

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Crack propagation in quasi-brittle materials using a FEM-VEM tracking algorithm

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Quasi-brittle materials mainly fail when, in the presence of specific stress scenarios, strains localize in narrow bands. Most of the computational strategies are developed in the framework of the finite element method (FEM) and can be divided into discrete crack models or smeared crack models. Discrete crack models introduce a strong or weak discontinuity along the inter-element boundaries or inside the element (intra-element discontinuity).

This work is inspired by the Augmented-FEM strategy [1]. A-FEM is a discrete crack model consisting in dividing the cracked element in two standard finite elements and a nonlinear interface where discontinuities localize. The additional degrees of freedom introduced to decompose the element are condensed at the equilibrium level, therefore are not present at the global level. An advancement of A-FEM was proposed in [2] and consisted in the use of a zero-thickness interphase model (IPH) [3] in place of the interface (ZTI), adding internal stresses and strains to the contact ones. Unlike ZTI models, IPH does not require a specific traction-displacement jump constitutive law and the constitutive laws adopted for IPH can correspond to those of bulk material, thus reducing the number of constitutive parameters.

Confirming advancements in [2], the innovative point of the present work resides in the description of the two sub-elements through the virtual element method (VEM) instead of FEM.

The VEM [4]-[5] is more flexible than standard FEM, since the element can be a polygon characterized by any number of edges, without constraints, with the ability to accurately deal with complex geometries, no need of a parent element, easy polynomial degree elevation, very good performances for distorted meshes.

The proposed crack tracking procedure starts with a discretization of the domain using standard finite elements. Known localization criteria and the spectral analysis of the fracture tensor built at the element level identify those elements crossed by a crack and crack orientation. Localized elements are then grouped into substructures, namely portions of the structure characterized by unique continuous cracks. Cracks are made continuous on the basis of simple heuristic criteria. Substructures are composed of virtual elements and IPHs representing discontinuities. At the global level, equilibrium is iteratively achieved by taking into account internal forces from substructures. These are solved in a VEM framework by imposing, as essential boundary conditions, displacements at nodes shared with the rest of the structure. Because the original element could be divided into very distorted sub-elements or non-standard elements, the VEM is more performant than the FEM. The main features of the adopted strategy are illustrated through benchmark examples.

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A non-smooth extrinsic cohesive zone model including contact and friction

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Cohesive zone models are a particularly high-fidelity way to model fracture propagation, although this accuracy comes at the cost of requiring high degrees of spatial and temporal refinement, which in turn means substantial computational demands. Cohesive zone models come in two basic flavours, intrinsic and extrinsic. Intrinsic models feature an initial elastic behaviour with crack opening, while extrinsic models are initially rigid. The extrinsic model family is universally recognised to be superior in dynamics due to its absence of spurious artificial compliance, but this comes at the cost of generally being more difficult to implement.

However, in instances of complex loading that cause cohesive zones to unload and then reload, this artificial compliance (and its associated numerical difficulties) can return, due to the elastic behaviour assumed in many models. As such, we aim to completely eliminate the pathologies of artificial compliance by eliminating the unload-reload elasticity from the formulation.

Due to the initial rigidity present in extrinsic cohesive zone models, using tools widely adopted in rigid-body mechanics is natural. We make use of non-smooth mechanics, a standard approach in rigid body and contact mechanics, to properly formulate an extrinsic mode I cohesive zone model that eliminates unload-reload elasticity, and also includes contact non-interpenetration within the formulation. After the construction of an implicit time-stepping schema, the discrete-in-time-and-space form of this model in dynamics can be written as a linear complementarity problem (LCP), which we are able to prove is well-posed and algorithmically dissipative (and symplectic in the absence of impacts), and is very efficient numerically [1]. We assign (and demonstrate) a physical meaning to this well-posedness, namely the absence of "solution jumps" given a sufficiently small time-step. We further demonstrate that a system that is ill-posed (exhibiting a solution jump) in quasi-statics becomes well-posed in dynamics, thus demonstrating the regularising effect of dynamics, even for slow loading rates.

Taking inspiration from classical non-smooth treatments of contact with friction [2], we extend our model to mixed mode I – mode II fracture, and we are also able to include the effects of friction within the model. We are once again able to write the problem as an LCP, for which we can exploit efficient numerical methods. As the problem is substantially more elaborate, we are only able to demonstrate a proof of the existence of the solution, but we are still able to show that the algorithm is dissipative numerically.

We are able to treat certain examples of academic interest from the literature [3], in some cases with orders-of-magnitude larger time-steps than comparable methods, by combining our monolithic LCP solver with the finite element method.

Finally, we highlight some potential future directions to extend the method, notably the extension to a fully mixed mode I – mode II – mode III model, and the possibility of capturing multiphysical effects using non-smooth mechanics techniques.

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Toughning effect of out-of-crack-path architected zones by apparition of snapback instability

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The rising of additive manufacturing has made it possible to build a new class of materials: architected materials. They are interesting for the industry because they can ally a relatively good resistance with a low density. In the context of this development, the question of the load-bearing capacity of these materials arises.

This work aims to tackle the problem of crack propagation in architected materials. This study focuses on remote effect of architected regions on crack propagation (Fig. 1). The question is to analyse how does the architecture modify the mechanical fields and has an effect on the crack tip and thus the propagation. This question is addressed in the framework of linear elastic quasi-static crack propagation, through finite element simulations with arc length algorithm [1]. The results are then validated using CT tests with 3D printed samples and digital image correlation for crack tracking [2].

The simulations allow bringing to light two important phenomena that can appear in this case: local slow down and snapback instability (Fig. 2). Local slow down refers to the fact that when the crack is between two architected zones, a larger displacement is required to propagate the crack than for the reference bulk sample.

The second phenomenon is the snap-back instability that appears at the end of the zone. In this work, we demonstrate that this is accompanied with an increase of dissipated energy by the crack propagation process. It means that the presence of the architected zone increases the total amount of external work needed to break the sample completely.

A parametric study is presented to understand the effect of the mechanical caracteristics of the architected zone on the two observed phenomena.

In this work, numerical models are used to prospect configurations and find toughening mechanisms made possible by architected materials. Experiments are used to validate that these phenomena effectively appear.

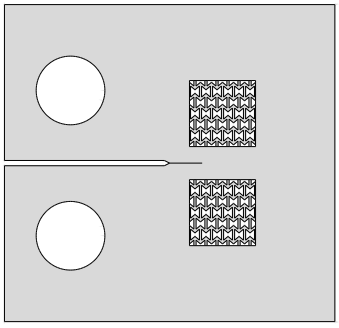

Figure 1: Geometry of the samples

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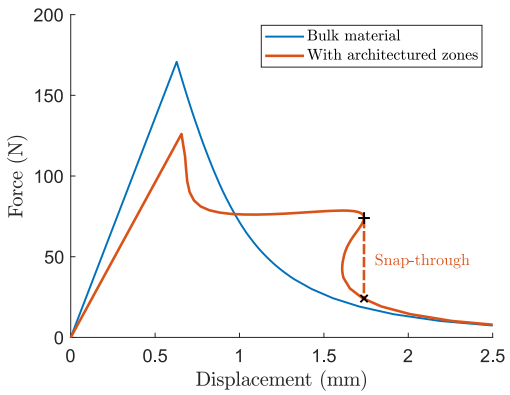

Figure 2: Numerically obtained loading curves

Variational Phase-field Fracture with Controlled Nucleation

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We describe recent work [1] on controlling nucleation in phase-field fracture. First we review the Γ-convergence of phase-field fracture to Griffith fracture, and describe how softening and nucleation occur when implementing phase-field models. An example is given of how this softening and nucleation can be completely stopped, while preserving crack growth and Γ–convergence. We then show how nucleation can locally be turned back on, based on any criterion, such as a stress threshold. Again, these modifications preserve Γ–convergence, and they can be applied to static, quasi-static, and dynamic models. Additionally, we describe why these modifications can be expected to improve the convergence of phase-field models.

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Free crack propagation through nonlocal modeling

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The fracture of brittle solids is a particularly interesting collective interaction connecting both large and small length scales. Apply enough stress or strain to a sample of brittle material and one eventually snaps bonds at the atomistic scale leading to fracture of the macroscopic specimen. In this talk a nonlocal mesoscopic fracture model is presented in which fractures emerge from the initial boundary value problem as part of the solution. The mesoscopic model eliminates the need for separate mathematical treatment of crack and intact material seen in classic (macroscopic) fracture models.

The nonlocal model carries details of the process zone seen at the mesoscopic length scale. In the limit of vanishing nonlocality, solutions of the model converge to solutions of the wave equation with evolving boundary formulated in Dal Maso and Toader [1], see [6].

The nonlocal dynamic initial value problem implicitly encodes the features of the classic model and delivers them in the limit of vanishing nonlocality [7].

In this talk the kinetic relation of LEFM is recovered from the nonlocal model noting that the same equation of motion applies everywhere in the body for the nonlocal model [5]. This is used to show that local power balance is given by the stationarity in time of the internal energy of a small domain containing the crack tip. The change in internal energy is shown to be the difference between the elastic energy flowing into the crack and the kinetic energy and stress work flux flowing into the domain. To leading order the stress work flux is precisely the rate of energy needed to create new surface. These results are obtained directly and exclusively from the dynamics governed by the nonlocal Cauchy equations of motion for a continuum body. This is the explicit connection between the nonlocal Cauchy equations of motion derived from double well potentials and the energy rate required to make new surface. For remote boundary loading we apply energy balance and pass to the local limit to recover the celebrated kinetic relation for the modern theory of dynamic fracture mechanics articulated in Freund [2], Ravi-Chandar [3].

Numerical simulations are given that illustrate the kinetic relation for roughly constant velocity traveling in a long strip. The crack velocity approaches steady state value of 0.6 which is consistent with the experimental result in Goldman et al. [4].

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Modeling Fracture of Tempered Glass Using an Eigenfracture Approach

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The failure mechanism of glass structures varies depending on several factors, which include the processing techniques used during the manufacture of glass-based elements (i.e. glass panels). To increase safety upon the fracture of glass structures, thermal or chemical treatment can be employed to produce toughened or tempered glass. Thermal tempering of glass is a process, where a glass pane is heated at high temperatures and is then cooled down rapidly, which induces residual compressive stresses at the outer surfaces and tensile stresses within the inner layer. This process influences the fracture pattern of glass panes significantly, where upon the initiation of fracture due to impact loading a thermally toughened pane breaks into relatively small fragments.

From a physical point of view, the dynamic process of glass fragmentation can be regarded as a result of multiple initiation of cracks, progressive crack branching and interlocking. The numerical modeling of this dynamic process has proven challenging due to various aspects. The emulation of the crack initiation and propagation criteria can be regarded as a demanding task, where different factors and comparatively complex scenarios (i.e. extremely small crack sizes) must be taken into account. Furthermore, the computational effort needed to model the process of fragmentation is generally considered as beyond the borders of practicality. Several approaches have been proposed in the literature to model the fragmentation process of brittle materials using numerical methods, such as the finite element method. These approaches include the introduction of a cohesive zone at the interface between finite elements, where a certain fracture criterion is met [1]. New surfaces are adaptively created as required based on a cohesive law, where certain nodes are duplicated along initially intact finite-element boundaries [1].

An eigenfracture approach is an approximation method proposed by [2] to simulate brittle fracture. The idea of eigenfracture has been implemented in the form of element erosion, which is an approach denoted by eigenerosion [3]. In order to predict the realistic crack kinematics, the representative crack element (RCE) method has been employed within an eigenerosion framewrok [4]. The RCE approach has advantages compared to other formulations, which are used to predict the crack-driving force (i.e. volumetric-deviatoric split) [4].

This contribution aims towards the finite-element simulation of fracture exhibited by annealed and tempered glass, under high loading rates. The eigenfracture method based on RCE approach [4] is adopted and further extended by taking into regard the emulation of brittle-fracture's evolution in the existence of residual stresses. In this work, the eigenfracture method is used to simulate crack branching in glass panes under tensile loading. Moreover, it is aimed to present the results of initial attempts to simulate the process of fragmentation, ranging from relatively big sizes of fragments (i.e. due to low residual stresses) to small sizes of fragments (i.e. caused by high levels of residual stresses). Finally, argumentations to improve the prediction capability of the developed approach and its efficiency are discussed.

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Comparison of a peridynamics and a phase-field approach to dynamic fracture

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Peridynamics and the phase-field fracture are two non-local methods to efficiently compute fracturing solids. While cracks in a solid are sharp two-dimensional hypersurfaces, the phase-field approach regularizes the material discontinuities with smooth transitions between broken and unbroken states. The evolution of the phase-field follows an equation where the driving forces of crack growth are derived from an energy minimization principle, typically based on an Ambrosio-Tortorelli type functional. Modifications allow accounting for the irreversible constraint of crack evolution and, especially important, for the asymmetry of fracture, i.e., cracks only grow under tensile loadings but not under compression [1,2]. Further modifications consider the evolution problem at finite strains using energy densities, which are polyconvex functions of the deformation, and/or at the regime of specific crack driving forces [2,3].

In this contribution, we focus particularity on pressure induced fracture. Different approximations will be presented, and dynamic finite element simulations of brittle fracture will be compared [3,4,5].

As an alternative to finite-element dicretizations, the particle based peridynamics will be discussed. The classical particle and bond-based peridynamics will be introduced and extended to a new geometrically precise framework, the continuum-kinematics-based peridynamics. This new formulation extends the classical method by introducing surface- or volume-based interactions, providing an exact geometrical method and a convenient way to simulate dynamic fracture. We will show that our recently introduced damage model [6] for the continuum-kinematics-based peridynamics effectively manages crack propagation under dynamic loading conditions with large deformations.

The main objective of this study is to illustrate the possibilities of dynamics fracture computations with the two methods. We will study the relationships of critical non-local fracture parameters and we will compare the phase-field fracture approach and the continuum-kinematics-based peridynamic framework in simulating wave propagation, superposition and cracking at critical states. The comparison will focus on the efficiency and accuracy of the two methods in capturing the critical fracture load and managing crack propagation under dynamic loading conditions with significant fragmentation.

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Applications of a micro-structured brittle damage model to laboratory tests on rocks

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A multiscale microstructured brittle damage model [1] is used to describe the behavior of confined rock materials.

Plane strain and triaxial tests conducted at the laboratory scale are simulated in terms of boundary value problems. Simulations reveal good predictive qualities of the model to describe the macroscopic features of specimens at failure. The microstructures, oriented in different directions, allow the localization of the macroscopic strain along straight lines, emerging at the macroscale in the form of shear bands.

The microstructured material model, characterized by recursive equidistant parallel cohesive-frictional faults, is fully defined by six elastic and inelastic material constants. The model was originally developed in a finite kinematics framework to simulate the dynamic behavior of confined brittle materials [2]. In linearized form, it has been extended and used for the simulation of in-field excavations [3]. The performance of the model in predicting the behavior of small scale rock tests in the laboratory, the object of the present study, has never been investigated.

In this study, we conduct numerical simulations of laboratory tests as boundary value problems, with the goal to show that the model is able to capture several important features observed in rocks, in particular the reduction of the overall stiffness for increasing deterioration of the material, fragile to ductile transition, strain localization, shear band formation, and more general size-effect.

The model, in all the numerical tests, has been able to describe the different responses of the sandstone, reproducing both the overall mechanical response and the failure patterns, in keeping with the typical brittle-to-ductile transition manifested by geological materials under confinement.
Remarkably, all the results have been obtained by using the same set of material parameters, with no need to tune them according to the particular loading condition examined [4].
This property is a natural outcome of the microstructured nature of the model that can be characterized by several length scales and does not suffer of mesh dependency when used in discretized domains.

We conclude that the brittle damage model in the linearized version is a very promising material model for geomechanical problems, especially considering the very small number (six) of characterizing material parameters.

References

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