

Advanced numerical modeling of fracture mechanics problems with the open-source FEniCS platform

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Abstract. Fracture mechanics is a fundamental field within solid mechanics that focuses on initiating and propagating cracks, which can lead to catastrophic mechanical failures in in-service components. Traditional Mechanics of Materials approaches often fall short of accurately predicting the behaviour of cracked materials, making analytical solutions impractical or even unattainable. Numerical modelling techniques, such as the finite element method, are employed to address this. However, high costs often restrict access to advanced engineering software for these simulations. Originally developed for simulating phase transformations, phase-field modelling has recently emerged as a powerful tool for overcoming longstanding challenges in the finite element formulation of fracture mechanics problems. This study presents the development of a computational tool for fracture simulation in anisotropic materials, implemented using the open-source FEniCS software. FEniCS is an open-source computational platform for solving partial differential equations via the finite element method. The effectiveness of this implementation will be assessed through numerical simulations, validated against benchmark experimental observations, including those documented in fracture challenge studies.

Keywords: Fracture mechanics, Phase field, FEniCS

1 Introduction

Phase-field models for fracture have gained prominence as a powerful alternative for simulating crack propagation, offering a diffuse representation of crack topology rather than tracking sharp discontinuities. Understanding crack initiation and propagation in anisotropic materials remains a significant challenge due to the influence of material inhomogeneity on the fracture path. In particular, when the specimen is subjected to pure mode I loading, a crack may deviate from a self-similar propagation direction if the material gradient is misaligned with the crack orientation. This misalignment introduces mode mixity at the crack tip, driven by the spatial variation in material properties, resulting in complex crack trajectories that are difficult to predict using conventional numerical techniques. Variational approaches based on energy minimization offer a robust framework for modeling fracture and present a compelling alternative to overcome the limitations of discrete methods [1]. Among these, the phase-field method has emerged as a powerful tool for simulating a wide range of fracture phenomena, including brittle fracture [2] ductile damage [3], fiber breakage and composite delamination [4], and hydrogen embrittlement [5],[6]. Building on this foundation, this work its a firs step to introduces a phase-field formulation

tailored for fracture in anisotropic materials, aiming to extend the method's success to systems with spatially varying properties and complex fracture behavior. Examples of such materials include fiber-reinforced composites, wood, and masonry, where directional mechanical behavior plays a critical role in fracture evolution. The objective of this work is to present a computational model in FEniCS [7] capable of representing anisotropic cracking in susceptible solids. FEniCS was chosen for this work because it is an open-source computing platform designed to solve partial differential equations using the finite element method. It is known for its user-friendly Python interface, flexibility, and efficiency. It supports various finite element types and custom function spaces and is optimized for high performance with parallel computing capabilities. Additionally, FEniCS offers extensive documentation and a supportive user community. We posit that code developed using FEniCS [8]can be readily accessed, thereby offering a highly efficient means of advancing scientific knowledge. This is particularly critical for understanding and modeling the mechanisms by which hydrogen degrades the ductility and fracture resistance of metals. In the following, we present the theoretical model grounded in physical governing equations, constitutive theory, and the phase-field method to capture the coupling between elasticity and damage effects. Preliminary results are also discussed.

2 General Theory

This study builds upon the theoretical foundations established in [5], [9], and [10], where the governing equations are derived using the principle of virtual power. The framework integrates key physical principles to model elasticity and damage within a thermodynamically consistent continuum approach. The material body consists of both isotropic and anisotropic elastic components. Deformation and fracture are coupled through a unified model that respects energy balance and constitutive consistency. The classical kinematic description is defined by the displacement field $\mathbf{u}$, while fracture and solute migration are represented by a scalar damage or phase-field variable ϕ, which transitions smoothly from $\phi = 0$ (undamaged) to $\phi = 1$ (fully fractured).

2.1 Basic Laws

The basic balance laws in its local form of a body β are defined below, following the [5] reference.

Linear momentum balance

$$\nabla \cdot \mathbf{S} + \mathbf{b} = \dot{\mathbf{p}} \quad \text{on} \quad \beta \quad \text{and} \quad \mathbf{S_n} = \mathbf{s}_{\partial\beta} \quad \text{on} \quad \partial\beta \tag{1}$$

Where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor, $\mathbf{b}$ body force, $\dot{\mathbf{p}}$ linear inertia momentum, $\mathbf{s}_{\partial\beta}$ is the boundary traction, $\mathbf{n}$ is the outward normal vector to the boundary. $\mathbf{S}$ is symmetric thanks to the frame-indifference of the internal power.

Phase-field method

The phase-field method for fracture is a robust computational approach that enables simulation of crack initiation, growth, and merging without explicitly tracking crack surfaces. It introduces a smooth scalar field ϕ, which transitions from 0 in intact regions to 1 in fully fractured zones, effectively regularizing the discontinuity of cracks. Rooted in Griffith's theory of brittle fracture, the method reformulates fracture as a variational problem that minimizes the total energy—comprising elastic strain energy and fracture surface energy. For a static, linear elastic body occupying a domain $\Omega \subset \mathbb{R}^2$, the boundary Γ is divided into Dirichlet (Γ_D) and Neumann (Γ_t) segments, with the closure defined as $\overline{\Omega} = \Omega \cup \Gamma$. Unlike classical fracture mechanics, which models cracks as sharp discontinuities along a surface Γ_c, the phase-field method uses the continuous field $\phi \in [0, 1]$ to represent damage. The crack zone's width is governed by a length scale parameter l, which controls spatial smoothing and resolution. Through

Γ-convergence, the regularized crack density functional $\Gamma_l(l,\phi)$ is shown to approximate the discrete crack energy as $l \to 0$, enabling accurate and efficient modeling of fracture processes.

$$\int_{\Gamma_c} G_c \, d\Gamma_c \approx \int_{\Gamma_c} G_c \, \Gamma_l(l,\phi) \, d\Omega = \int_{\Gamma_c} G_c \left(\frac{1}{2l}\phi^2 + \frac{l}{2}|\nabla\phi|^2 \right) d\Omega \tag{2}$$

The approximated crack surface energy (1) can be incorporated into the bulk energy to define the total potential energy of the solid as

$$\Psi = \int_{\Omega} \left((1-\phi)^2 \psi(\varepsilon) + G_c \Big(\frac{1}{2l}\phi^2 + \frac{l}{2}|\nabla\phi|^2 \Big) \right) d\Omega \tag{3}$$

where the term $(1-\phi)^2$ represents the degradation of the stored elastic energy as damage evolves within the material. The strain energy density of the undamaged isotropic linear elastic material solid is expressed as a function of the strain tensor is given by,

$$\psi(\boldsymbol{\varepsilon}) = \frac{1}{2}\lambda(\mathrm{tr}\boldsymbol{\varepsilon})^2 + \mu\,(\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}) = \frac{1}{2}\lambda(\mathrm{tr}\boldsymbol{\varepsilon})^2 + \mu\,\mathrm{tr}(\boldsymbol{\varepsilon}) \tag{4}$$

where, $\boldsymbol{\varepsilon}$ denotes the strain tensor, and λ, μ are the Lame's parameters. The strain tensor is related to the displacement field $\boldsymbol{u}$ through the standard kinematic relation:

$$\boldsymbol{\varepsilon} = \mathrm{sym}\,\nabla\boldsymbol{u} \tag{5}$$

where $\mathrm{sym}\,\nabla\boldsymbol{u} = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^\top)$. By taking the first variation of Equation (2) and applying the Gauss theorem, the following coupled field equations are obtained, valid for any arbitrary variations of the kinematic fields $\delta\boldsymbol{u}$ and $\delta\phi$.

$$(1-\phi)^2\boldsymbol{\sigma}\cdot\boldsymbol{n} = 0 \quad in \quad \Omega \tag{6}$$

$$G_c\left(\frac{1}{l}\phi + l\,\Delta\phi\right) - 2(1-\phi)\psi(\varepsilon) = 0 \quad in \quad \Omega \tag{7}$$

Here, (σ) denotes the Cauchy stress tensor. For a traction $\boldsymbol{T}$, the natural boundary conditions readily follow as

$$(1-\phi)^2\boldsymbol{\sigma}\cdot\boldsymbol{n} = \boldsymbol{T} \quad on \quad \Gamma \tag{8}$$

$$\nabla\phi\cdot\boldsymbol{n} = 0 \quad in \quad on \quad \Gamma \tag{9}$$

2D Isotropic Elastic Material

A 2D isotropic elastic material is a simplified model where mechanical properties are identical in all directions, making its stress–strain response direction-independent. The material behaves elastically, meaning it returns to its original shape once the applied stress is removed, as long as the stress remains within the elastic limit. The analysis is restricted to two dimensions, typically under plane stress or plane strain conditions. In the plane strain case, the constitutive equations are adjusted to reflect zero strain in the out-of-plane direction. Using Voigt notation, the constitutive relation for a 2D isotropic elastic material is expressed as:

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{33} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ 2\varepsilon_{xy} \end{bmatrix}$$

where

$$C_{11} = C_{22} = \frac{E}{1-\nu^2} \qquad C_{12} = \frac{E\nu}{1-\nu^2} \qquad C_{33} = \frac{E}{2(1+\nu)}$$

with E is Young's modulus and ν is Poisson's ratio.

2D Anisotropic Elastic Material

In the case of anisotropic materials, meaning materials with direction-dependent properties, exhibit complex fracture behavior. This anisotropy significantly influences crack paths and fracture toughness, particularly when considering the material's orientation and thickness. So for a 2D anisotropic elastic material, the generalized Hooke's law relates stress and strain via the stiffness tensor. In 2D (plane stress or plane strain), the generalized Hooke's law for a 2D anisotropic elastic material or constitutive equations can be written as:

$$\sigma_{ij} = \sum_{k=1}^{2}\sum_{l=1}^{2} C_{ijkl}\varepsilon_{kl}$$

where the stiffness matrix $\mathbf{C}$ in Voigt notation, which simplifies the tensor notation for symmetric stress and strain tensors. In Voigt notation, this reduces to:

$$\begin{bmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{xy}\end{bmatrix} = \begin{bmatrix}C_{11} & C_{12} & C_{16}\\ C_{12} & C_{22} & C_{26}\\ C_{16} & C_{26} & C_{66}\end{bmatrix}\begin{bmatrix}\varepsilon_{xx}\\ \varepsilon_{yy}\\ 2\varepsilon_{xy}\end{bmatrix}$$

where σ_{ij}: components of the stress tensor ε_{kl}: components of the strain tensor C_{ijkl}: components of the stiffness tensor (anisotropic, so all components may be nonzero) and $C_{11}, C_{12}, C_{22}, C_{16}, C_{26}, C_{66}$ are the independent stiffness constants for the most general 2D anisotropic material. Note that for engineering shear strain, the factor is used in the third component of the strain vector.

Finite element implementation

The finite element method is used to solved the coupled system of equations (4). We follow the hybrid model by Ambati et al. [16]; to maintain resistance in compression and during crack closure we reformulate (4b) as

$$G_c\left(\frac{1}{l}\phi + l\,\Delta\phi\right) - 2(1-\phi)H^{+} \;=\; 0 \tag{10}$$

where H^{+} is the so-called history variable field, which is defined as

$$H^{+} \;=\; \max\phi^{+}(\varepsilon(t)) \quad in \quad \Gamma_{t\in[0.\tau]} \quad \text{with} \quad \psi^{+}(\boldsymbol{\varepsilon}) = \frac{1}{2}K(\text{tr})^2\boldsymbol{\varepsilon})^2 + \mu\,(\boldsymbol{\varepsilon}^{dev} : \boldsymbol{\varepsilon}^{dev}) \tag{11}$$

following Amor et al. [17]. Here, $\langle a\rangle = \frac{1}{2}(a+|a|)$ and K is the bulk modulus. The resulting weak form can be obtained by considering the dimensional trial $(\mathcal{U};\mathcal{P})$ and test spaces $(\mathcal{V};\mathcal{Q})$. Let $\mathcal{W}$ include the linear displacement field and phase field variable:

$$(\mathcal{U},\mathcal{P}) \;=\; \{(u,v)\in[C^0(\Omega)]^d : (u,v)\in[\mathcal{W}(\Omega)]^d \subseteq [\mathcal{H}^1(\Omega)]^d\} \tag{12}$$

$$(\mathcal{P},\mathcal{L}) \;=\; \{(\phi,q)\in[C^0(\Omega)]^d : (\phi,q)\in[\mathcal{W}(\Omega)]^d \subseteq [\mathcal{H}^1(\Omega)]^d\} \tag{13}$$

The system of equations can be readily obtained upon applying the standard Bubnov-Galerkin procedure. In the absence of remote tractions and body forces, one can find $u\in U$ and $\phi\in P$ for all $v\in V$ and $q\in Q$ by solving.

$$\int_{\Omega}\Big\{(1-\phi)^2\boldsymbol{\sigma}(\boldsymbol{u}) : \boldsymbol{\varepsilon}(\boldsymbol{v})\Big\}\,d\Omega \;=\; 0 \tag{14}$$

$$\int_{\Omega}\Big\{\nabla q\cdot\nabla\phi G_c l + q\Big(\frac{G_c}{l} + 2H^{+}\Big)\phi - 2H^{+}q\Big\}d\Omega \;=\; 0 \tag{15}$$

The system is solved using a staggered scheme, where the displacement field and phase-field variable are updated sequentially to improve numerical stability and simplify handling of nonlinear coupling. Leveraging FEniCS—an open-source finite element framework—offers significant advantages through its symbolic differentiation capabilities. This allows direct implementation of the weak form of the governing equations (Equation 2.1), eliminating the need for manual derivation of residuals and tangent matrices. FEniCS streamlines the development of phase-field fracture models, enabling researchers to focus on physical modeling and parameter tuning. It also supports rapid prototyping and testing of alternative formulations, including different degradation laws, crack-driving mechanisms, and boundary conditions.

3 Metodology

The main steps of the simulation procedure are illustrated using a well-established benchmark: a rectangular plate subjected to uniaxial tension (see Fig. 2a).

Mesh Generation

The first step is to construct the mesh. With this aim ew have used the open-source software Gmsh [18] to generate the mesh and export it in .msh format. This file can then be converted to .xml using the dolfin-convert utility, allowing it to be imported nto the Python script via the FEniCS Mesh command.

Material Properties

Material parameters are manually defined within the script. To validate our implementation, we compare the results with those reported by Miehe et al. [5], using the following material properties:

- Young's modulus: $E = 210$ GPa
- Poisson's ratio: $\nu = 0.3$
- Critical energy release rate: $G_c = 2.7$ MPa.mm

Simulations are performed for two different values of the internal length scale parameter l, to investigate its effect on the fracture response.

Boundary Conditions

Boundary conditions are defined by identifying the relevant edges and applying Dirichlet conditions to both the displacement field $\boldsymbol{u}$ and the phase-field variable ϕ. Following the setup in [5], the bottom edge of the plate is clamped, while a prescribed vertical displacement u_r is applied to the top edge, simulating remote loading. This configuration is illustrated in Fig. xxx.

4 Numerical results

The study investigates fracture behavior under mixed-mode loading, where complex stress states influence crack path and propagation rate—critical factors in damage mechanics and fracture analysis. As shown in Figure 1, the configuration features a notched plate with slanted crack propagation, introducing stress asymmetry and enabling exploration of anisotropic damage effects. Figure 2 presents the finite element mesh used in the simulations. Local refinement is applied near the anticipated damage zone to accurately capture stress gradients and crack-tip behavior while maintaining computational efficiency. This meshing strategy ensures reliable predictions of crack initiation and growth, effectively balancing precision and performance in modeling anisotropic fracture.

Three cases were analyzed, with the first focusing on an isotropic material. Figure X shows the evolution of the damage variable for this case, using a material characterized by Young's modulus $E = 210 \times 10^6$ and Poisson's ratio $\nu = 0.3$. The simulation captures the progressive degradation under

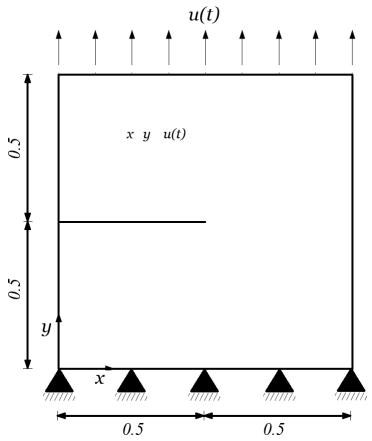


Figure 1. Configuration setup

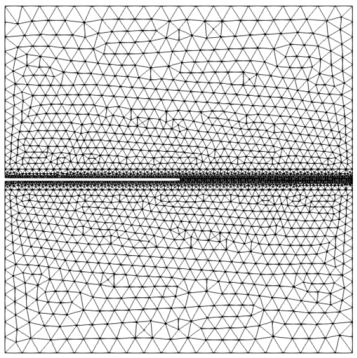


Figure 2. Mesh refinement

mechanical loading, revealing the spatial distribution and growth of damage. The boundary conditions consist of a fully clamped base, restricting all movement, while a time-dependent vertical displacement is applied to the top edge over the interval $t \in [0, 1]$. This gradual loading enables a smooth stress evolution, allowing precise observation of damage initiation and propagation throughout the structure. To validate the FEniCS implementation under different material configurations, two additional analyses

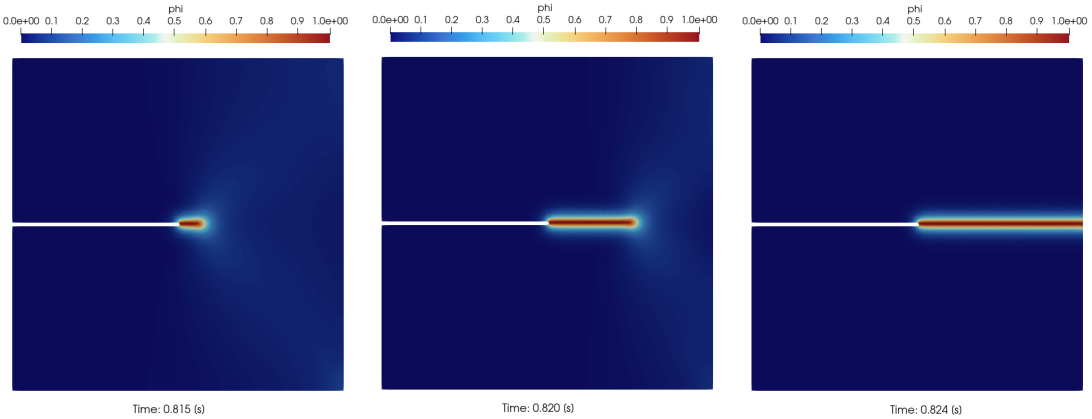


Figure 3. Crack approximation and length scale parameter (Miehe, Welschinger and Hofacker, 2010b)

were performed. Case II examines an isotropic material with adjusted properties—Young's modulus $E = 190 \times 10^3$ and Poisson's ratio $\nu = 0.4$ to evaluate the sensitivity of damage evolution to changes in stiffness and lateral contraction. Case III explores an orthotropic material with directional stiffness, defined by $E_x = 200 \times 10^3$, $E_y = 100 \times 10^3$, $\nu_{xy} = 0.3$, and shear modulus $G_{xy} = 0.6$. This setup enables analysis of anisotropic damage behavior and its effect on crack propagation. The results from all three cases are presented in the following plot, illustrating how variations in material anisotropy and stiffness influence damage patterns and mechanical response. Preliminary results reveal that the constitutive model strongly influences the reaction–displacement response. With the cleavage plane oriented at 90° to the horizontal axis and vertical loading applied, fracture consistently follows the cleavage direction due to its inherent weakness. All cases exhibit elastic–brittle behavior, characteristic of unstable crack propagation.The observed damage patterns resemble those from uniaxial tension tests, marked by localized bands. This reflects a competition between mode I crack opening and anisotropic cleavage effects. As anisotropy increases, the cleavage orientation increasingly dictates the fracture path, intensifying damage localization and steering crack growth.

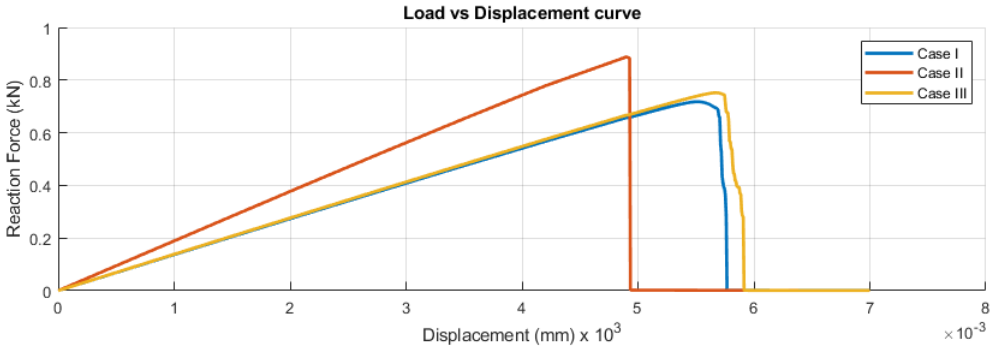


Figure 4. Reaction vs. Displacement curves for Case I, Case II, and Case III)

5 Next Steps

This work presents initial findings on anisotropic brittle fracture modeling using a variational phase-field approach. The introduction of an anisotropic stiffness tensor enables directional sensitivity in material response, while a hybrid numerical scheme—combining direct and iterative solvers—ensures robust and efficient computation. The model effectively captures key anisotropic effects, particularly the non-convex nature of fracture energy with respect to orientation. Although it does not fully replicate zig-zag crack patterns observed experimentally, it demonstrates crack kinking behavior driven by directional stiffness degradation. These results highlight the need for careful parameter calibration and establish a strong foundation for advancing anisotropic fracture modeling in engineering contexts.

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