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ADVANCES ON HIGH-FIDELITY PHASE-FIELD MODELS FOR FRACTURE MECHANICS OF QUASI-BRITTLE MATERIALS AND INTERFACES

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Abstract. The phase field approach to fracture has attracted much attention since its first application to brittle fracture in 1998, due to its unique simulation potential and easy implementation. The present work aims at reviewing the most recent advances to render it a high-fidelity computational method able to quantitatively solve problems of high engineering relevance. Specifically, the following major issues are addressed: (i) quantitative validation of the phase field models in relation to experimental tests involving complex crack patterns; (ii) extension of the basic formulation within a multi-phase field framework to simulate damage in compression and crushing failure in addition to tensile cracking; (iii) interplay between bulk fracture and cohesive interface delamination in composites, for statics and dynamics. Conclusions highlight perspective research directions.

1 INTRODUCTION

This article reviews the progress made over the recent years at the IMT School for Advanced Studies Lucca in the field of computational fracture mechanics, achieved through extensive collaborations with established research groups at the University of Seville, University of Girona, University of Hannover, University of Trento and Politecnico di Torino, which led to several publications on theory and numerics aiming at making the phase field approach to fracture a reliable engineering tool.

Starting from the seminal work by Ambrosio and Tortorelli [1] on the mathematical treatment of the functionals typically used in image segmentation, the methodology was exploited by Francfort and Marigot in 1998 [2] to treat fracture mechanics problems, leading to the so-called variational approach to fracture, also called phase-field. A significant impulse to the method was given by Miehe et al. [3], who made a consistent progress on its numerical implementation in the finite element method within a thermo-dynamically consistent framework. The variational approach to fracture retrieves the well-established linear elastic fracture mechanics (LEFM) scenario as a limit case for a vanishing internal length scale [2], and includes the key features of nonlocal damage mechanics [4, 5] for a finite one. The great potential in simulating crack growth without the need of invoking mesh refinement algorithms has attracted a wide attention by the scientific community, which extended the basic method and made further improvements upon it, see e.g. [6–10] and the references therein given.

Today, the methodology is in the position to become a widely recognized standard method for 2D and 3D fracture mechanics simulations. However, it still requires further validation and developments to become an engineering tool able to provide fully reliable quantitative predictions [11]. This article reviews some important steps undertaken to make further progress on phase field modelling of fracture. Section 2 addresses the experimental assessment and validation of the two most popular versions of the phase field method in relation to a wide testing campaign on PMMA material. Section 3 addresses the generalization of the basic method to deal with damage in compression in addition to fracture in tension, and their interplay. Finally, Sec. 4 discusses its consistent integration with other popular nonlinear fracture mechanics formulations like the cohesive zone model (CZM), which can be effectively exploited for the existing material interfaces, both in statics and dynamics. Conclusions highlight future research directions in the area of phase field modelling of fracture.

2 THE PHASE FIELD APPROACH TO BRITTLE FRACTURE IN A NUTSHELL AND ITS EXPERIMENTAL VALIDATION

The variational approach to brittle fracture is set up through the definition of the following free energy functional [2]:

$$\Pi(\mathbf{u},\Gamma) = \int_{\Omega\backslash\Gamma} \psi^e(\boldsymbol{\varepsilon})\,\mathrm{d}\Omega + \int_{\Gamma_f} \mathcal{G}_c\,\mathrm{d}\Gamma \quad (1)$$

where $\psi^e(\boldsymbol{\varepsilon})$ is the elastic energy density that depends upon the strain field $\boldsymbol{\varepsilon}$, and $\mathcal{G}_c$ is the fracture energy.

To simulate damage only in tension, the following decomposition of the energy density is introduced:

$$\psi^e(\boldsymbol{\varepsilon}, s) = \{(1-s)^2 + k\}\psi^e_+(\boldsymbol{\varepsilon}) + \psi^e_-(\boldsymbol{\varepsilon}) \quad (2)$$

where the positive and negative parts of the energy density are defined in [3] and the term $(1-s)^2 + k$ is the degradation function dependent on the phase field variable s $(0 \leq s \leq 1)$.

A crack density functional γ is adopted to smear out damage in tension, which has the following expressions for the AT1 and the AT2 models [10]:

$$\gamma(s,\nabla s) = \begin{cases} \dfrac{3}{8l}s + \dfrac{3l}{8}|\nabla s|^2, & \text{AT1} \\ \dfrac{1}{2l}s^2 + \dfrac{l}{2}|\nabla s|^2, & \text{AT2} \end{cases} \quad (3)$$

where l has the meaning of a regularization length. According to $\Gamma-$convergence considerations, the regularized functional reads:

$$\Pi(\mathbf{u}, s) = \int_\Omega \psi^e(\boldsymbol{\varepsilon}, s)\,\mathrm{d}\Omega + \int_\Omega G_c\gamma\,\mathrm{d}\Omega \quad (4)$$

In deriving the weak form from the functional (4), the irreversibility condition of damage is implemented in the AT1 model by introducing a penalty term [12], while a strain history function is adopted for the AT2 model [3].

Numerically, the problem can be solved either monolithically [13] or by introducing a staggered scheme [14]. The latter implies an alternate minimization of the weak form associated to the phase field variable for frozen displacements, and then the minimization of the weak form associated to the mechanical field for a frozen phase field variable. A convergence criterion based on the norm of the two fields within the iterative step should be introduced to guarantee convergence, as rigorously implemented in [14]. In case of a single pass staggered scheme, without iterations, the accuracy of the post-peak prediction is in fact highly deteriorated.

Alternative phase field formulations are those by Feng and Wu [15] and by Fei and Choo [16], which were exploited in [11]. Those models do consider different strain energy decompositions from the canonical ones discussed above and introduce other forms of degradation function with additional parameters. The model parameters' identification for those formulations is an open issue.

The above AT1 and AT2 phase field models for fracture have been carefully scrutinized in [14] in relation to a novel wide photoelastic experimental campaign on PMMA samples, subject to tension and compression, and containing circular holes, V-notches and sharp notches.

Following the prescriptions in [10], the internal length scale l for the AT1 and the AT2 models have been preliminary estimated through the following formulae which relate l to the tensile strength $\sigma_{\max}$ obtained from the peak load at failure in a uniaxial tensile test simulation, the Young's modulus E, and the fracture toughness G_c:

$$l = \begin{cases} \dfrac{3}{8}\dfrac{G_c E}{\sigma_{\max}^2}, & \text{(AT1)}, \\[2ex] \dfrac{27}{256}\dfrac{G_c E}{\sigma_{\max}^2}, & \text{(AT2)}, \end{cases} \tag{5}$$

For PMMA, Eq.(5) leads to $l = 0.174$ mm for the AT1 and $l = 0.049$ mm for the AT2 model, respectively. The application of the phase field approach to fracture to notched compact tests with two holes, with tiny sharp notches inserted in the holes, see Fig.1, were considered to be particularly challenging in terms of crack pattern and force-displacement evolution to be simulated using the existing fracture mechanics tools.

The comparison between experimental results and the AT1 and AT2 model predictions are illustrated in Fig.2 for one of the several benchmark tests analyzed in [14]. The AT1 model accurately predicted the peak load, point (1), just using the value of $l = 0.174$ mm estimated from the uniaxial test formula, while the simulated post-peak response was overestimating the measured experimental load. On the other hand, the AT2 model systematically predicted higher values of the peak load when using $l = 0.049$ mm according to Eq.(5). The blue curve shown in Fig.2 was obtained by increasing l to 0.2 mm, which allowed to capture very well the whole post-peak response, in spite of the underestimation of the peak load.

Figure 1: Fractured compact test specimen made of PMMA with an initial notch and 2 circular holes, each one having a tiny sharp notch [14].

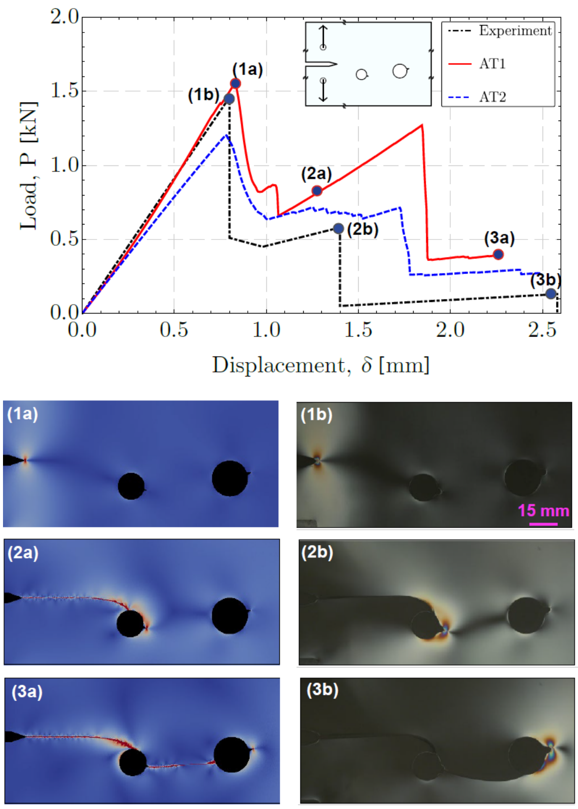


Figure 2: Load vs. displacement curves of the compact test in Fig.1 and plots comparing the crack path and the photoelastic fringes from simulation (left panels) and experiments (right panels).

Additional results in [14] regarded other specimen geometries and loading conditions (three-point bending test with a notched beam and an internal hole; plate tested in compression with an internal circular hole and two horizontal sharp notches inserted in the hole) and showed that the AT1 model has good predictive capabilities, just using the value of l identified from uniaxial tensile tests. On the other hand, the AT2 model generally requires the use of different values of l from those identified from uniaxial tests. Although this preliminary result should be confirmed by a more extensive investigation involving also other materials, it may imply that the AT2 model requires the repetition of the task of model parameters' identification when applied to different test geometries and loading conditions.

3 A MULTI-PHASE FIELD APPROACH TO SIMULATE FRACTURE AND CRUSHING

Brittle materials in compression exhibit a specific type of failure which involves material crushing, which is a mechanism of energy dissipation physically distinct from tensile fracture and, as such, it cannot be simulated within the phase field models summarized in Sec. 2. Experimental uniaxial compressive tests on concrete specimens [17] highlight the occurrence of a mechanism of material crushing which leads to a specific energy dissipation in compression which is one order of magnitude higher than in tension. Moreover, they show the existence of an internal length scale corresponding to the band where energy dissipation takes place. Based on those considerations, the *overlapping crack model* for damage in compression was pioneeringly proposed by Carpinteri et al. [18], in close analogy with the *cohesive zone model* in tension. The idea was to model the effect of diffused energy dissipation during crushing events as an equivalent single crack in compression where the energy dissipated is the result of the work done by compressive tractions multiplied by a fictitious material compenetration.

Although successfully applied to concrete specimens in compression [19,20] and to beams in three-point bending [21] with a single tensile/overlapping crack, there is indeed the need of an energetically rigorous fracture mechanics model that could be applied not only at the global scale, but also at the mesoscale.

Hence, in order to improve the capability of the phase field approach to fracture to simulate also damage in compression, which is precluded by the classical way damage is introduced by the tensorial split, a multi-phase field formulation has been proposed in [22] by adding an additional independent damage field in compression, with its own evolution law, to simulate crushing failure in addition to tensile fracture.

The variational approach to brittle fracture and material crushing is therefore set up through the definition of the following free energy functional:

$$\begin{aligned}\Pi(\mathbf{u},\Gamma) = \int_{\Omega\backslash\Gamma} \psi^e(\boldsymbol{\varepsilon})\,\mathrm{d}\Omega + \int_{\Gamma_f} \mathcal{G}_c\,\mathrm{d}\Gamma \\ + \int_{\Gamma_c} \mathcal{G}_{c,c}\,\mathrm{d}\Gamma\end{aligned} \tag{6}$$

where $\psi^e(\boldsymbol{\varepsilon})$ is the elastic energy density that depends upon the strain field $\boldsymbol{\varepsilon}$, and $\mathcal{G}_c, \mathcal{G}_{c,c}$ are, respectively, the fracture energy in tension and the crushing energy in compression.

To account for different damage mechanisms, the following decomposition of the energy density is introduced [22]:

$$\begin{aligned}\psi^e(\boldsymbol{\varepsilon}, s_1, s_2) = \{(1-s_1)^2 + k\}\psi^e_+(\boldsymbol{\varepsilon}) \\ + \{(1-s_2)^2 + k\}\psi^e_-(\boldsymbol{\varepsilon})\end{aligned} \tag{7}$$

where the positive and negative parts of the energy density are defined as in [3], with two independent phase field variables s_1 and s_2, the former to depict damage in tension, and the latter to simulate damage in compression.

A crushing density functional γ_c is also introduced in addition to the crack density functional γ, to smear out damage not only in tension but also in compression [22]:

$$\begin{aligned}\Pi(\mathbf{u}, s_1, s_2) = &\int_\Omega \psi^e(\boldsymbol{\varepsilon}, s_1, s_2)\,\mathrm{d}\Omega \\ &+ \int_\Omega G_c \gamma(s_1, \nabla s_1)\,\mathrm{d}\Omega + \\ &+ \int_\Omega G_{c,c}\gamma_c(s_2, \nabla s_2)\,\mathrm{d}\Omega\end{aligned} \tag{8}$$

where the AT2 expression has been employed in analogy with tensile fracture:

$$\gamma_c(s_2, \nabla s_2) = \frac{1}{2l_c} s_2^2 + \frac{l_c}{2}|\nabla s_2|^2 \tag{9}$$

where the second regularization length scale l_c is introduced, which is an additional parameter independent from l.

This radically new formulation has been tested in [22] to simulate meso-scale models of cylindrical and prismatic concrete specimens under compression, modelled as a brittle matrix with embedded aggregates, see Fig.3 and [22] for the model parameters selected to simulate the behaviour of normal strength concrete.

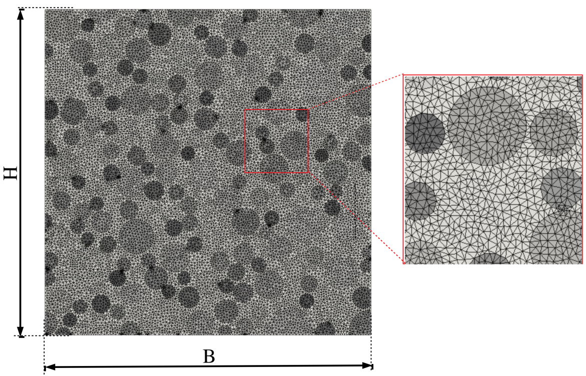


Figure 3: 2D meso-scale model of a concrete cubic specimen.

The deformed mesh at failure and the contour plots of the phase field variable s_1 associated to fracture and of the phase field variable s_2 associated to crushing are shown in Figs.4 and 5, for a 2D model of a cubic specimen tested under uniaxial compression with low or high lateral confinement.

In case of low lateral confinement (Fig.4), sub-vertical cracks tend to propagate and induce a splitting failure mode. Damage in compression is therefore quite limited in its spread.

A high lateral confinement, on the other hand, is leading to shear band formation with also crushing observed along the shear band (Fig.5).

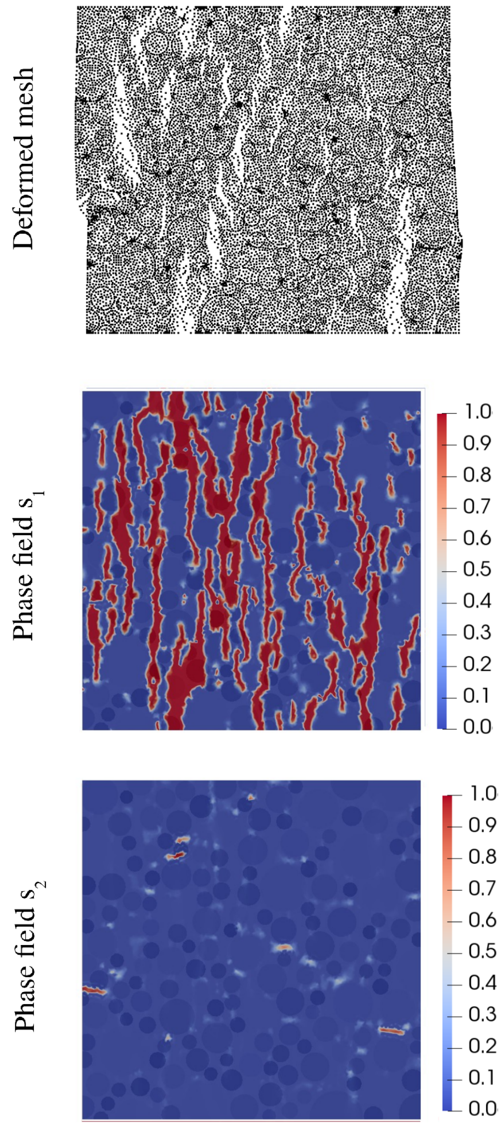


Figure 4: Splitting failure of cubic specimens with low lateral confinement: damage in tension (s_1) and in compression (s_2).

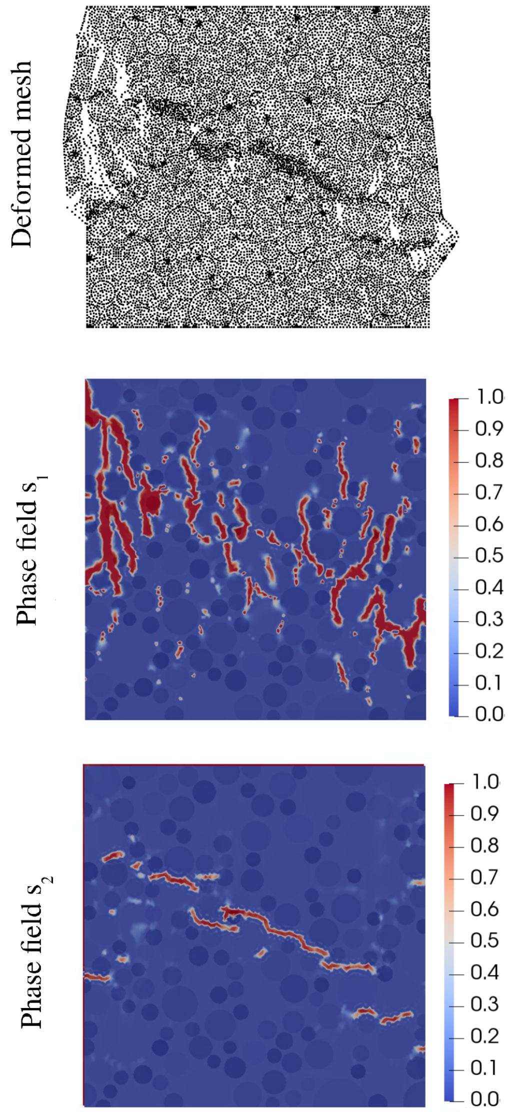


Figure 5: Diagonal failure of cubic specimens with high lateral confinement: damage in tension (s_1) and in compression (s_2).

In addition to the realistically predicted damage patterns, the model also predicts quantitative values for the compressive strength from the computed peak load of the force displacement curves. The predicted cubic compressive strength, R_c, is shown in Fig.6 vs. the tangent elastic modulus in compression, E^*, for a series or random simulations considering low lateral confinement (low friction between the concrete specimen and the steel platens), and for a high lateral confinement (high friction). In line with the trends reported in the literature [23], the average cubic strength over the tested random population (black solid line) in the case of high confinement is significantly higher than for low confinement (dashed line). For more results on the effect of the specimen aspect ratio, see [22] for the analysis analogous simulations on cylindrical specimens.

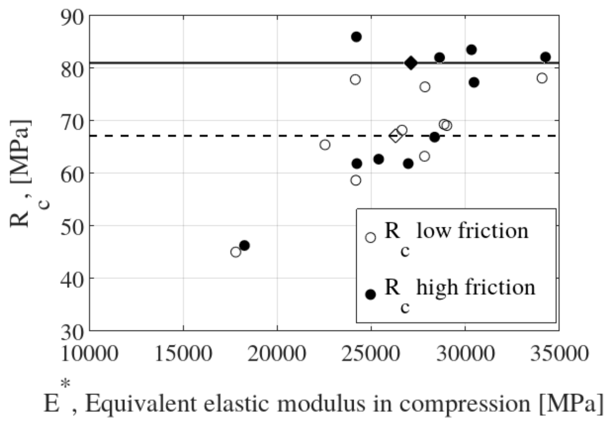


Figure 6: Predicted cubic compressive strength R_c vs. equivalent elastic modulus in compression, E^*. The solid line refers to the average response of the simulated population for high confinement, while the dashed line refers to the low confinement case.

4 ADVANCED APPLICATIONS TO INTERFACE MECHANICAL PROBLEMS IN STATICS AND DYNAMICS

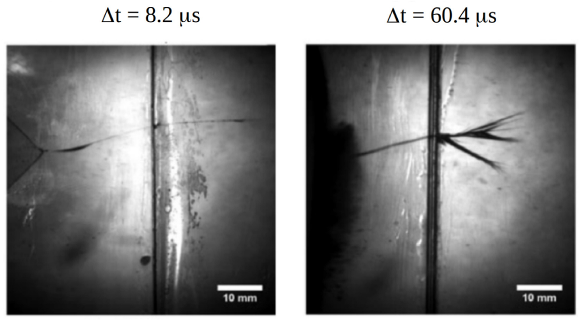
The potential of using the phase field approach to fracture to simulate damage in the bulk in conjunction with the cohesive zone model (CZM) to address damage scenarios at pre-existing material interfaces has been pioneeringly proposed in [24]. For the first time, the combined use of these two nonlinear fracture mechanics models was able to retrieve the fundamental LEFM solution by He and Hutchinson [25] concerning the different possible crack growth paths for a crack meeting a bi-material interface. Moreover, results in [25] were also extended in [24] to quasi-brittle interfaces, providing a comprehensive theoretical framework based on dimensional analysis for the interpretation of the interplay between bulk and interface fracture events.

The methodology proposed in [24] has been further applied to laminates [26–28] and fiber-reinforced materials [29, 30], to model complex scenarios involving bulk fracture and interface decohesion in heterogeneous materials and components.

The extension of the formulation to dynamic loading has been published in [31], including both inertia terms for the bulk and for the finite thickness adhesive interface, through a rigorous derivation of the Hamiltonian principle. An implicit monolithic full Newton-Raphson incremental-iterative scheme was employed to integrate the equations of motion in time and solve the strong nonlinear mechanical problem involved by the simultaneous presence of two forms of nonlinearities, one due to phase field fracture and one related to interface decohesion ruled by a CZM under mixed-mode conditions.

Representative applications regarded the problem of crack propagation through interfaces in a Borosilicate glass and a glass ceramic experimentally tested in [32] under the action of a projectile impacting on the specimen and inducing dynamic crack growth from the initial notch. Such a crack, as one can see from their recorded high-speed camera images in Fig.7, meets the bi-material interface and its further propagation in the second material layer is delayed depending on the thickess of the adhesive layer.

The use of thin adhesives, which corresponds to a stiffer interface bonding, leads to a very short time delay Δt before the crack travels into the second layer. On the other hand, thick adhesives lead to a much bigger time delay Δt, which is caused by the higher compliance of the interface and it can be explained as a result of a significant amount of energy dissipated during interface decohesion in mixed-mode. Moreover, crack branching in the second material layer is also observed in this scenario.



(a) Interface thickness 0.2 mm (b) Interface thickness 1.0 mm

Figure 7: Experimental evidences of the effect of the interface thickness on dynamic crack propagation through layered materials (both in terms of time delay for the crack to penetrate in the second layer and crack path), images adapted from [32].

Numerical simulations were able to capture the different crack pattern experimentally observed in the two cases (see Figs.8 and 9), in addition to the different amount of decohesion experienced by the interface and the very different time delay before the occurrence of crack penetration into the second layer.

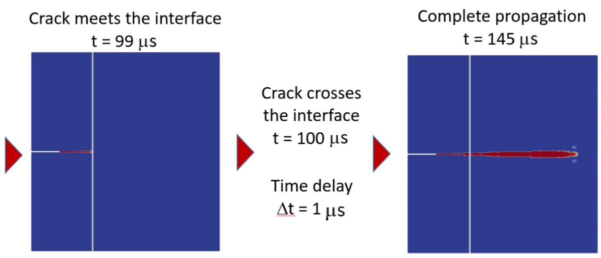


Figure 8: Simulation of the crack path and time elapsed during crack propagation for a thin adhesive interface.

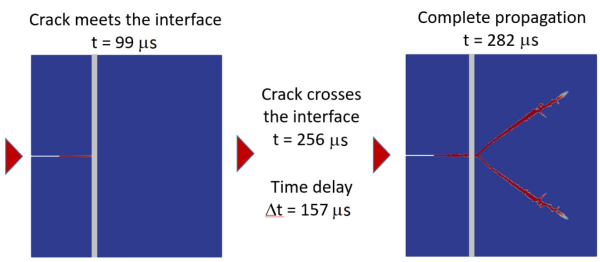


Figure 9: Simulation of the crack path and time elapsed during crack propagation for a thick adhesive interface.

5 CONCLUSION

The reliability of the phase field approach to fracture has been shown to be significantly increased over time, becoming nowadays a quantitative tool able to predict with good accuracy force-displacement curves in addition to the excellent qualitative matching with the experimentally observed crack paths. In this regard, multi-phase field formulations, although computationally more expensive, are very promising, since they feature physical models very important in real applications, such as crushing failure in addition to tensile cracking. Moreover, the methodology is prone to be used for advanced coupled problems involving thermoelasticity [33, 34], or even contact-induced fracture events, as recently addressed in [35] with a sophisticate interface model with roughness for the contacting interface combined with the phase field approach for the simulation of cracking in the bulk. Eventually, implementations of the phase field approach to fracture in finite element formulations for structural analysis, such as plates and shells [36, 37] and solid shell finite elements [38], open also the path to the simulation of high-fidelity fracture mechanics problems in civil structures.

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