RESEARCH ARTICLE

A dissipation-based path-following technique for the phase-field approach to brittle and ductile fracture

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2448, 3001 Leuven, Belgium. Email:
jef.wambacq@kuleuven.be**Summary**

This paper presents a dissipation-based path-following technique for the phase-field approach to brittle and ductile fracture. This technique allows computing the post-peak response of solids loaded by external forces and snap-backs in the softening stage. By controlling the dissipated energy during loading, the solid is prevented from unloading elastically, and an equilibrium branch with a continuous increase of dissipated energy is followed. Because solids can dissipate in both tension and compression, a discontinuous equilibrium path can be obtained. To avoid this occurrence, two novel techniques are presented, which ensure a continuous equilibrium path for which the solid is either in tension or compression. In addition, the thermodynamic constraints present in the phase-field model are rigorously solved using an interior-point method. In order to allow for simultaneous dissipation due to both plastic and damage mechanisms, the governing equations are solved monolithically. The presented method is tested on four benchmark problems, and it is observed that by tracing snap-backs, time-discontinuous evolutions are avoided, which restores energy balance and enhances the convergence of the monolithic scheme.

KEYWORDS:

phase-field models, brittle fracture, ductile fracture, path-following techniques, dissipation-based, monolithic scheme

1 | INTRODUCTION

In order to capture the post-peak response of solids and structures, most studies on the phase-field approach to quasi-static fracture^{1–13} rely on displacement-controlled simulations. As such, simulations involving solids loaded by external forces are precluded, and snap-backs in the post-peak regime of the equilibrium path cannot be captured. Consequently, time-discontinuous jumps can arise, e.g. during brutal crack propagation, and the total energy of the system may not be conserved. Under such conditions, rate-dependent phenomena, which are not included in the present formulation, are likely to occur¹⁴. To capture the post-peak response of solids loaded by external forces or snap-backs in the softening stage of the equilibrium path, path-following techniques can be adopted. However, due to the localized nature of cracks and their complex topologies, the choice of an adequate path-following constraint is not straightforward.

In the framework of classical non-linear finite element analyses, several path-following techniques have been developed. Wempner¹⁵ and Riks¹⁶ suggested to augment the governing equations of problems with elastic instabilities with an auxiliary path-following constraint, in terms of a load multiplier that scales the external load. Later, Crisfield¹⁷ and Ramm¹⁸ proposed a partitioned procedure, similar to the displacement control method of Batoz and Dhatt¹⁹. As such, symmetry of the augmented

system of equations is restored, and more efficient solution procedures can be adopted. The aforementioned path-following constraints are purely geometrical, involve all degrees of freedom, and typically lead to elastic unloading when applied to problems with softening material behavior²⁰. To approach this issue in fracture problems with softening behavior, de Borst²¹ proposes to use the crack-mouth opening displacement as a controlling parameter. This method is more robust but requires a priori knowledge of the crack topology, such as the subset of the degrees of freedom that determines the crack width. Alternatively, Chen and Schreyer²² propose an adaptive path-following technique, where only the degrees of freedom that determine the strain components of the most distorted point of the solid are controlled. Geers^{23,24} generalizes the methods where a subset of degrees of freedom are controlled, and defines the path-following constraints of Crisfield¹⁷ and Ramm¹⁸ in adaptive subspaces of all degrees of freedom. Later, Pohl et al.²⁰ suggested an adaptive path-following scheme, where the controlling parameter is based on zones where damage is increasing. Alternatively, Gutiérrez²⁵ proposes to control the dissipated energy caused by damage. This was extended by Verhoosel et al.²⁶ to problems governed by plasticity and geometrically non-linear damage. As such, no a priori knowledge is required on the structural behavior and adaptive controlling parameters are not necessary. A further extension of the method is presented by Paullo and Roehl²⁷ who combine multiple path-following constraints and solve the over-determined system using the least squares method. This leads to an unsymmetric system of equations for which Mejia et al.²⁸ propose a partitioned procedure, where the least squares method is only used to determine the load multiplier while the displacements are computed from a symmetric system of equations. A comparison of the performance of various path-following constraints was conducted by Fayezioghani et al.²⁹.

In order to combine path-following techniques with the phase-field approach to brittle and ductile fracture, the governing equations of the phase-field model need to be augmented with a path-following constraint. The governing equations of variational phase-field models are typically obtained from the minimization of a non-convex energy functional subject to thermodynamic constraints, leading to a system of variational inequalities¹¹. In the literature, various algorithms have been presented to minimize the energy functional. Staggered schemes exploit the convexity of the functional with respect to each individual argument, resulting in an algorithmic decoupling of the governing equations^{3,10,30}. Alternatively, monolithic schemes solve the coupled problem for all arguments simultaneously^{5,8,12,31} and enable the use of more complex path-following constraints because multiple fields can be controlled concurrently.

In order to capture snap-backs in a quasi-brittle one-dimensional bar, Vignollet et al.³² solve the weak form of the governing equations monolithically and augment the system of equations with the dissipation-based path-following constraint of Gutiérrez²⁵. Later, May et al.³³ extended this approach by controlling the internal energy in non-dissipative parts of the loading. In addition, the proposed technique was applied to a two-dimensional example of a plate with an eccentric hole modeled with the phase-field approach to brittle fracture. In both cases, irreversibility of the crack phase-field is imposed with a history field, as proposed by Miehe et al.³. As such, the variational structure of the problem is destroyed, and the system of equations is no longer symmetric. Alternatively, Luege et al.³⁴ propose an augmented Lagrangian to enforce irreversibility and augment the weak forms of the optimality conditions with a dissipation-based path-following constraint. Singh et al.³⁵ depart from the monolithic scheme, and solve for a displacement multiplier by controlling the fracture surface area using a staggered scheme, while imposing irreversibility using the history field. As such, the symmetry of the equations is not affected by the history field. Later, Wu³⁶ applied this technique to the so-called unified phase-field theory⁹ to capture snap-backs in the equilibrium path of a direct tension test on a concrete specimen.

An algorithm that allows capturing snap-backs in equilibrium paths of solids governed by the phase-field approach to ductile fracture, where energy is dissipated by both damage and plastic mechanisms, has not been presented in the literature yet. In order to control the energy dissipated in both mechanisms, the evolution equations of damage and plasticity must be solved simultaneously. Therefore, this paper presents an extension of the monolithic scheme for brittle and ductile fracture proposed by Wambacq et al.¹³ to include a dissipation-based path-following constraint that accounts for both plastic and damage dissipation. As such, an equilibrium path with a continuous increase of dissipated energy is followed, ensuring energy balance and avoiding time-discontinuous jumps and brutal crack propagation, which is expected to result in a more robust monolithic scheme.

The outline of the paper is as follows. In section 2, the notation and the governing equations are presented. Next, in section 3, a novel monolithic scheme for brittle and ductile phase-field problems is augmented with a path-following constraint. In addition, two techniques are presented to differentiate between dissipation in tension and compression. Section 4 presents four numerical examples, illustrating the results of the proposed method using various path-following constraints and both techniques to differentiate between dissipation in tension and compression. The examples show that the proposed method allows tracing the entire equilibrium path, and it is observed that by avoiding time-discontinuous jumps, the total energy is conserved and the convergence of the monolithic scheme is enhanced. Finally, in section 5, the work is concluded.

2 | NOTATION AND GOVERNING EQUATIONS

In this section, the governing equations of brittle and ductile fracture are obtained using the energetic formulation for rate-independent systems³⁷. First, the energetic quantities that describe how a solid stores internal energy and dissipates energy are discussed. This is followed by statements of energy balance, a dissipation inequality and a stability condition, which are used to obtain the governing equations. In a third step, these equations are discretized in time, which results in an incremental system of equations that is suitable for numerical implementation. In addition, the incremental equations are augmented with a path-following constraint, which allows capturing snap-backs in the equilibrium path. The system of equations is discretized using finite elements, resulting in a constrained system of discrete non-linear equations.

2.1 | Energetic quantities

Consider a solid domain $\Omega \subset \mathbb{R}^3$ with boundary $\Gamma \subset \mathbb{R}^3$, on which displacements $\bar{\mathbf{u}}(\mathbf{x}, t) = \mathbf{0} \in \mathbb{R}^3$ are imposed on the homogeneous Dirichlet boundary $\Gamma_D \subset \Gamma$, and a traction $\lambda(t)\bar{\mathbf{l}}(\mathbf{x}) \in \mathbb{R}^3$ is applied on the Neumann boundary $\Gamma_N \subset \Gamma$, such that $\Gamma_D \cup \Gamma_N = \Gamma$ and $\Gamma_D \cap \Gamma_N = \emptyset$. For the sake of simplicity, no non-homogeneous Dirichlet boundary conditions are considered, but the framework can be straightforwardly extended to incorporate displacement loading on Γ_D . The load multiplier $\lambda : T \rightarrow \mathbb{R}_+$ scales the external load over a time interval $T := [0, t_{\max}]$ and, without loss of generality, the spatial distribution $\bar{\mathbf{l}}(\mathbf{x})$ of the traction is chosen such that the load multiplier is always positive. The deformation process is quasi-static. In addition, all deformations are assumed to be infinitesimally small, except in certain localized regions. In this setting, the aim of this paper is to present an algorithm which allows computing the displacement field $\mathbf{u} : \Omega \times T \rightarrow \mathbb{R}^3$, the plastic strain tensor $\epsilon^p : \Omega \times T \rightarrow \mathbb{R}_{\text{dev}}^{3 \times 3}$, and the crack phase-field $\alpha : \Omega \times T \rightarrow [0, 1]$ in the solid, where $\mathbb{R}_{\text{dev}}^{3 \times 3} := \{\mathbf{e} \in \mathbb{R}_{\text{sym}}^{3 \times 3} \mid \text{tr } \mathbf{e} = 0\}$ is the set of symmetric and deviatoric second-order tensors. The constitutive behavior of the solid is governed by two energetic quantities, which are elaborated below.

The internal potential energy density describes the elastic energy stored in the solid, and is given by a non-convex state function that reads

$$\psi(\epsilon(\mathbf{u}), \epsilon^p, \alpha) := g(\alpha)\psi^{e+}(\epsilon(\mathbf{u}), \epsilon^p) + \psi^{e-}(\epsilon(\mathbf{u}), \epsilon^p), \quad (1)$$

where $\epsilon := \nabla^s \mathbf{u} = \frac{1}{2}(\nabla \otimes \mathbf{u} + \mathbf{u} \otimes \nabla)$ is the second-order infinitesimal strain tensor, and $g(\alpha) := (1 - \alpha)^2$ is the usual quadratic degradation function. For notational simplicity, explicit dependence on space and time has been omitted in equation (1), as will be done hereinafter. In order to introduce asymmetric behavior in tension and compression, the internal potential energy density is decomposed into degradable and non-degradable parts, denoted by $\psi^{e+}(\epsilon, \epsilon^p)$ and $\psi^{e-}(\epsilon, \epsilon^p)$, respectively. Various definitions of the degradable and non-degradable parts are presented in the literature^{1,2,38,39}. Similar to the ductile fracture models presented in^{10,40,41}, the volumetric-deviatoric decomposition proposed by Amor et al.¹ is used, where the elastic energy density is decomposed as

$$\begin{cases} \psi^{e+}(\epsilon, \epsilon^p) := \frac{1}{2}K \langle \text{tr}(\epsilon^e) \rangle_+^2 + G(\epsilon_{\text{dev}}^e : \epsilon_{\text{dev}}^e), \\ \psi^{e-}(\epsilon, \epsilon^p) := \frac{1}{2}K \langle \text{tr}(\epsilon^e) \rangle_-^2, \end{cases} \quad (2)$$

where K is the bulk modulus, G is the shear modulus, $\langle \square \rangle_{\pm} := \frac{1}{2}(\square \pm |\square|)$ is the ramp function, and $\epsilon_{\text{dev}}^e : \Omega \times T \rightarrow \mathbb{R}_{\text{dev}}^{3 \times 3}$ is the deviatoric part of the elastic strain tensor $\epsilon^e := \epsilon - \epsilon^p$. From the decomposed energy density, the stress tensor is determined as follows:

$$\sigma(\epsilon, \epsilon^p, \alpha) = g(\alpha) \frac{\partial \psi^{e+}}{\partial \epsilon}(\epsilon, \epsilon^p) + \frac{\partial \psi^{e-}}{\partial \epsilon}(\epsilon, \epsilon^p). \quad (3)$$

As such, the deviatoric stress tensor is always degraded. This is a convenient feature for the ductile fracture model adopted in this paper, where plasticity is driven by deviatoric stresses.

The total internal potential energy describes the elastic energy stored in the solid, and reads

$$\mathcal{E}(\mathbf{u}, \epsilon^p, \alpha) := \int_{\Omega} \left(g(\alpha)\psi^{e+}(\epsilon(\mathbf{u}), \epsilon^p) + \psi^{e-}(\epsilon(\mathbf{u}), \epsilon^p) \right) d\mathbf{x}. \quad (4)$$

The dissipation potential describes the rate of dissipated energy in the solid, and is given by a convex homogeneous function of degree one with respect to the rates of the internal variables. The following dissipation potential, corresponding to the model

of Alessi et al.⁴, is adopted:

$$\phi(\dot{\kappa}, \dot{\alpha}, \nabla \dot{\alpha}; \kappa, \alpha, \nabla \alpha) := \underbrace{g(\alpha)\sigma^p \dot{\kappa}}_{\text{plastic diss.}} + \underbrace{g'(\alpha)\sigma^p \kappa \dot{\alpha}}_{\text{coupling}} + \underbrace{w'(\alpha)\dot{\alpha} + \eta_d^2 \nabla \alpha \cdot \nabla \dot{\alpha}}_{\text{damage diss.}}, \quad (5)$$

where $\kappa : \Omega \times T \rightarrow \mathbb{R}_+$ is the equivalent plastic strain evolving as $\dot{\kappa} := \sqrt{2/3} \|\dot{\epsilon}^p\|$, σ^p is the yield strength, and $\eta_d := \ell_d \sqrt{2w_0}$ is a length scale that governs the localization of damage in which ℓ_d is the damage characteristic length with the units of length. In equation (5), $g'(\alpha)$ and $w'(\alpha)$ denote the derivative of $g(\alpha)$ and $w(\alpha)$ with respect to α , respectively, where $w(\alpha)$ is the dissipation due to the local damage evolution for which two options are typically adopted:

$$w(\alpha) := \begin{cases} w_0 \alpha & \text{AT-1,} \\ w_0 \alpha^2 & \text{AT-2.} \end{cases} \quad (6)$$

In this function, w_0 is a local damage dissipation constant. The AT-1 model leads to an elastic regime before the onset of damage or plasticity, whereas in the AT-2 model, damage starts to evolve immediately upon loading^{7,11}. In addition, in the absence of plasticity, the dissipation potential for ductile fracture (5) reduces to the dissipation potential for brittle fracture, where w_0 and η_d can be expressed in terms of the fracture toughness G_c and the damage characteristic length ℓ_d . As such, w_0 and η_d are given by $w_0 = 3G_c/(8\ell_d)$ and $\eta_d = \sqrt{3G_c\ell_d}/2$ in the case of the AT-1 model, and $w_0 = G_c/(2\ell_d)$ and $\eta_d = \sqrt{G_c\ell_d}$ in the case of the AT-2 model.

The dissipative power functional describes the total dissipated power in the solid, and is defined as

$$\mathcal{R}(\dot{\kappa}, \dot{\alpha}; \kappa, \alpha) = \int_{\Omega} \phi(\dot{\kappa}, \dot{\alpha}, \nabla \dot{\alpha}; \kappa, \alpha, \nabla \alpha) d\mathbf{x}. \quad (7)$$

The dissipated energy corresponding to the dissipation potential in equation (5) is a state function⁴². As such, the dissipated energy between two states $\{\kappa_0, \alpha_0\}$ and $\{\kappa_1, \alpha_1\}$ at t_0 and t_1 can be computed analytically, and reads

$$D(\kappa_0, \alpha_0, \kappa_1, \alpha_1) := \int_{t_0}^{t_1} \mathcal{R}(\dot{\kappa}, \dot{\alpha}; \kappa, \alpha) d\tau = \int_{\Omega} \left[\left(g(\alpha_1)\sigma^p \kappa_1 + w(\alpha_1) + \frac{1}{2}\eta_d^2 \|\nabla \alpha_1\|^2 \right) - \left(g(\alpha_0)\sigma^p \kappa_0 + w(\alpha_0) + \frac{1}{2}\eta_d^2 \|\nabla \alpha_0\|^2 \right) \right] d\mathbf{x}, \quad (8)$$

where $\|\square\| := \|\square\|_{\ell^2}$ is the Euclidean norm.

2.2 | Energetic formulation

The equations governing brittle and ductile fracture are obtained using the energetic framework of Mielke³⁷, based on an energy balance and a stability condition. In addition, a dissipation inequality is included to guarantee physically sound results. Energy balance and the dissipation inequality correspond to reformulations of the first and second laws of thermodynamics, while stability further restricts the set of possible solutions¹⁴.

Energy balance

A process is energetically consistent if the following energy balance holds:

$$\mathcal{E}(\mathbf{u}, \epsilon^p, \alpha) + D(\kappa_0, \alpha_0, \kappa, \alpha) = \mathcal{E}(\mathbf{u}_0, \epsilon_0^p, \alpha_0) + \int_{\Gamma_N} \int_0^t \lambda \bar{\mathbf{t}} \cdot \dot{\mathbf{u}} d\tau dS, \quad (9)$$

where the state corresponding to $t = 0$ is denoted by a zero in subscript, and the contribution of the work supplied by tractions on the Dirichlet boundary vanishes because only homogeneous Dirichlet boundary conditions are considered. From energy balance, the plastic flow rule and the consistency conditions for the plastic and damage evolution equations can be obtained (see e.g. Alessi et al.⁴).

Dissipation inequality

A process is thermodynamically consistent if the rate of dissipated energy is non-negative:

$$\phi(\dot{\kappa}, \dot{\alpha}, \nabla \dot{\alpha}; \kappa, \alpha, \nabla \alpha) \geq 0 \quad \text{in } \Omega \times T. \quad (10)$$

Similar to other brittle and ductile phase-field models^{2,4,7}, it is assumed that crack healing cannot occur and, consequently, the rate of the crack phase-field variable α is non-negative. Hereafter, the monotonicity constraint $\dot{\alpha} \geq 0$ will be enforced, which, together with $\dot{\kappa} = \sqrt{2/3} \|\dot{\epsilon}^p\|$, renders the local part of the dissipation potential (5) non-negative. However, due to the presence of the gradient term in the dissipation potential, it can only be guaranteed that the damage dissipation inequality holds in integral form, which corresponds to a physically sound non-decreasing crack surface.

Stability

Various stability conditions are formulated in the literature. A thorough discussion on this topic in the context of rate-independent processes is given by Mielke and Roubíček⁴³. Hereafter, local stability is considered. This implies that, at a given time step, the solution is such that the corresponding energy state attains a local minimum. Therefore, for all admissible variations $\{\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}\}$ in the neighborhood of the current state, there exists $\bar{h} > 0$ such that

$$\mathcal{E}(\mathbf{u}, \epsilon^p, \alpha) \leq \mathcal{E}(\mathbf{u} + h\tilde{\mathbf{u}}, \epsilon^p + h\tilde{\epsilon}^p, \alpha + h\tilde{\alpha}) + \mathcal{D}(\kappa, \alpha, \kappa + h\sqrt{2/3}\|\tilde{\epsilon}^p\|, \alpha + h\tilde{\alpha}) - \int_{\Gamma_N} \lambda \tilde{\mathbf{t}} \cdot h\tilde{\mathbf{u}} \, dS, \quad \forall h \in [0, \bar{h}], \quad (11)$$

where the virtual fields $\{\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}\}$ explicitly consider the homogeneous Dirichlet boundary conditions, and irreversibility of the crack phase-field $\tilde{\alpha} \geq 0$ (see e.g. Marigo et al.⁷ in the case of brittle fracture). The function spaces for all fields and their admissible variations read

$$\begin{aligned} \mathcal{U} &:= \{\mathbf{u} \in BD(\Omega; \mathbb{R}^3) \mid \mathbf{u} = \mathbf{0} \text{ on } \Gamma_D\}, & \tilde{\mathcal{U}} &:= \mathcal{U}, \\ \mathcal{B} &:= \mathcal{M}(\Omega \cup \Gamma_D; \mathbb{R}_{\text{dev}}^{3 \times 3}), & \tilde{\mathcal{B}} &:= \mathcal{B}, \\ \mathcal{D} &:= H^1(\Omega; [0, 1]), & \tilde{\mathcal{D}} &:= H^1(\Omega; \mathbb{R}_+), \end{aligned} \quad (12)$$

where $BD(\Omega; \mathbb{R}^3)$ is the space of bounded deformations, $\mathcal{M}(\Omega \cup \Gamma_D; \mathbb{R}_{\text{dev}}^{3 \times 3})$ is a space of Radon measures, and $H^1(\Omega; \mathbb{R})$ is the usual Sobolev space. Since no plastic hardening or non-local plastic effects are considered, shear bands can develop and sharp discontinuities can occur in the displacement field, which cannot be resolved in a Sobolev space. Therefore, the space of bounded deformations and a space of Radon measures is introduced for the displacement field and plastic strain tensor, respectively. A detailed discussion on this topic is given by Dal Maso et al.⁴⁴ or Bartels et al.⁴⁵. The set $\{\mathbf{u}, \epsilon^p, \alpha\} \in \mathcal{U} \times \mathcal{B} \times \mathcal{D}$ contains admissible displacement fields and internal variables, considering kinematic admissibility of the displacement field and boundedness of the crack phase-field. Similarly, the set $\{\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}\} \in \tilde{\mathcal{U}} \times \tilde{\mathcal{B}} \times \tilde{\mathcal{D}}$ contains admissible virtual displacement fields and internal variables, as well as the monotonicity constraint on the crack phase-field.

A first-order stability condition is obtained by replacing the right-hand side of (11) by the first-order terms of its Taylor expansion:

$$\delta \mathcal{E}(\mathbf{u}, \epsilon^p, \alpha)(\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}) + \mathcal{R}(\sqrt{2/3}\|\tilde{\epsilon}^p\|, \tilde{\alpha}; \kappa, \alpha) - \int_{\Gamma_N} \lambda \tilde{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, dS \geq 0, \quad \forall \{\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}\} \in \tilde{\mathcal{U}} \times \tilde{\mathcal{B}} \times \tilde{\mathcal{D}}, \quad (13)$$

where $\delta \mathcal{E}(\square)(\tilde{\square})$ is the Gâteaux derivative of $\mathcal{E}(\square)$ in the direction of $\tilde{\square}$. It can be shown that (13) provides the yield criteria, which together with energy balance and the dissipation inequality fully define the evolution problem.

2.3 | Governing equations in incremental form

In order to obtain a numerical step-by-step time integration of the governing equations, the time interval T is discretized using a pseudo-time step parameter $n \in \mathbb{N} \cup \{0\}$. A quantity evaluated at the previous time step t_n , where all variables are known, is denoted with a subscript n , while a quantity evaluated at t_{n+1} is written without a subscript for brevity.

Ductile phase-field model

The first-order stability condition (13) can be modified using an indicator function, explicitly considering the boundedness of the crack phase-field as follows:

$$\delta \mathcal{E}(\mathbf{u}, \epsilon^p, \alpha)(\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}) + \mathcal{R}(\sqrt{2/3}\|\tilde{\epsilon}^p\|, \tilde{\alpha}; \kappa, \alpha) - \int_{\Gamma_N} \lambda \tilde{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, dS + \int_{\Omega} \partial I_{[\alpha_n, 1]}(\alpha) \tilde{\alpha} \, d\mathbf{x} \geq 0, \quad \forall \{\tilde{\mathbf{u}}, \tilde{\epsilon}^p, \tilde{\alpha}\} \in \tilde{\mathcal{U}} \times \tilde{\mathcal{B}} \times \tilde{\mathcal{D}}, \quad (14)$$

where $I_C(\square)$ is an indicator function that equals 0 if $\square \in C$ and $+\infty$ otherwise, and, $\partial I_C(\square)$ is the subdifferential of the indicator function, which gives 0 if $\square \in C \setminus \partial C$, $\mathbb{R}_-$ if $\square \in \partial C$, and $\emptyset$ otherwise. By adding the indicator function to the

functional, the admissible space for the crack phase-field is no longer constrained and its function space is relaxed to $H^1(\Omega; \mathbb{R})$. As such, the governing equations in weak form read

$$\left\{ \int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^p, \alpha) : \nabla^s \tilde{\mathbf{u}} \, d\mathbf{x} - \lambda \int_{\Gamma_N} \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, dS = 0, \quad \forall \tilde{\mathbf{u}} \in \tilde{\mathcal{U}}, \right. \quad (15a)$$

$$\left\{ \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \|\boldsymbol{\sigma}_{\text{dev}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^p, \alpha)\| + g(\alpha) \sigma^p \right) \|\tilde{\boldsymbol{\epsilon}}^p\| \, d\mathbf{x} \geq 0, \quad \forall \tilde{\boldsymbol{\epsilon}}^p \in \tilde{\mathcal{B}}, \right. \quad (15b)$$

$$\left\{ \int_{\Omega} \left[\left(g'(\alpha)(\psi^{\epsilon^+}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^p) + \sigma^p \kappa) + w'(\alpha) + \partial I_{[\alpha_n, 1]}(\alpha) \right) \tilde{\alpha} + \eta_d^2 \nabla \alpha \cdot \nabla \tilde{\alpha} \right] \, d\mathbf{x} \ni 0, \quad \forall \tilde{\alpha} \in \tilde{\mathcal{D}}, \right. \quad (15c)$$

where the optimality conditions are satisfied for $\boldsymbol{\sigma} : \tilde{\boldsymbol{\epsilon}}^p = \|\boldsymbol{\sigma}_{\text{dev}}\| \|\tilde{\boldsymbol{\epsilon}}^p\|$. Herein, $\boldsymbol{\sigma}_{\text{dev}}$ is the deviatoric part of the stress tensor $\boldsymbol{\sigma}$ given in equation (3), and the equivalent plastic strain is given by $\kappa = \kappa_n + \sqrt{2/3} \|\boldsymbol{\epsilon}^p - \boldsymbol{\epsilon}_n^p\|$.

In the incremental setting, the plastic strain tensor can be eliminated from the system in (15) by using an incremental form of the associative flow rule, i.e. $\boldsymbol{\epsilon}^p = \boldsymbol{\epsilon}_n^p + \sqrt{3/2} \hat{\mathbf{n}}(\kappa - \kappa_n)$, where $\hat{\mathbf{n}} := \boldsymbol{\sigma}_{\text{dev}} / \|\boldsymbol{\sigma}_{\text{dev}}\|$ is the direction of the plastic flow. Similar to the classical radial return method⁴⁶, an implicit scheme is used, where the direction of the plastic flow at the stress state at t_{n+1} and the trial state coincide, i.e. $\hat{\mathbf{n}} = \boldsymbol{\sigma}_{\text{dev}}^{\text{tr}} / \|\boldsymbol{\sigma}_{\text{dev}}^{\text{tr}}\|$, where $\boldsymbol{\sigma}_{\text{dev}}^{\text{tr}} := 2g(\alpha)G(\boldsymbol{\epsilon}_{\text{dev}} - \boldsymbol{\epsilon}_n^p)$ is the deviatoric part of the trial stress tensor. In addition, the equivalent plastic strain must be constrained to $[\kappa_n, +\infty)$. As such, the weak form of the plastic yield criterion (15b) is recast as

$$\int_{\Omega} \left[\left(-\sqrt{\frac{3}{2}} \|\boldsymbol{\sigma}_{\text{dev}}^{\text{tr}}(\boldsymbol{\epsilon}, \alpha; \boldsymbol{\epsilon}_n^p)\| + g(\alpha)(\sigma^p + 3G(\kappa - \kappa_n)) + \partial I_{[\kappa_n, +\infty)}(\kappa) \right) \|\tilde{\boldsymbol{\epsilon}}^p\| \right] \, d\mathbf{x} \ni 0, \quad \forall \tilde{\boldsymbol{\epsilon}}^p \in \tilde{\mathcal{B}}. \quad (16)$$

Using the definition of the subdifferential of indicator functions, the system of variational inequalities (15a), (15c) and (16) is cast in the following system of variational equalities, similar to the procedure in Mang et al.⁴⁷:

$$\left\{ \begin{aligned} & \int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^p(\kappa), \alpha) : \nabla^s \tilde{\mathbf{u}} \, d\mathbf{x} - \lambda \int_{\Gamma_N} \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, dS = 0, \quad \forall \tilde{\mathbf{u}} \in \tilde{\mathcal{U}}, \\ & \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \|\boldsymbol{\sigma}_{\text{dev}}^{\text{tr}}(\boldsymbol{\epsilon}, \alpha; \boldsymbol{\epsilon}_n^p)\| + g(\alpha)(\sigma^p + 3G(\kappa - \kappa_n)) - \lambda_{\kappa} \right) \|\tilde{\boldsymbol{\epsilon}}^p\| \, d\mathbf{x} = 0, \quad \forall \tilde{\boldsymbol{\epsilon}}^p \in \tilde{\mathcal{B}}, \\ & \int_{\Omega} \left[\left(g'(\alpha)(\psi^{\epsilon^+}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^p(\kappa)) + \sigma^p \kappa) + w'(\alpha) - (\lambda_{\alpha_1} - \lambda_{\alpha_2}) \right) \tilde{\alpha} + \eta_d^2 \nabla \alpha \cdot \nabla \tilde{\alpha} \right] \, d\mathbf{x} = 0, \quad \forall \tilde{\alpha} \in \tilde{\mathcal{D}}, \end{aligned} \right. \quad (17)$$

where λ_{κ} , λ_{α_1} and λ_{α_2} act as Lagrange multipliers satisfying the following KKT conditions:

$$\left\{ \begin{aligned} & \lambda_{\kappa}(\kappa - \kappa_n) = 0, \quad \lambda_{\kappa} \geq 0, \quad (\kappa - \kappa_n) \geq 0, \\ & \lambda_{\alpha_1}(\alpha - \alpha_n) = 0, \quad \lambda_{\alpha_1} \geq 0, \quad (\alpha - \alpha_n) \geq 0, \\ & \lambda_{\alpha_2}(1 - \alpha) = 0, \quad \lambda_{\alpha_2} \geq 0, \quad (1 - \alpha) \geq 0. \end{aligned} \right. \quad (18)$$

Path-following constraint

In order to determine the load multiplier λ , the governing equations (17) and (18) are augmented with a path-following constraint. Hereafter, a displacement control and a dissipation-based path-following constraint will be adopted.

The displacement control path-following constraint is used to trace the non-dissipative parts of the equilibrium path, and reads

$$c(u^{\beta}(\mathbf{x}); u_n^{\beta}(\mathbf{x}), \Delta s) := u^{\beta}(\mathbf{x}) - u_n^{\beta}(\mathbf{x}) - \Delta s = 0, \quad (19)$$

where $\Delta s \in \mathbb{R}$ is a user-defined step size and $u^{\beta}(\mathbf{x})$ is the displacement at a position $\mathbf{x}$ in the direction of $\beta \in \{x, y, z\}$. The presented framework can be straightforwardly generalized to other path-following constraints^{16–18} for the case of geometrical instabilities, where the equilibrium path can show snap-backs in non-dissipative parts.

The dissipation-based path-following constraint controls the dissipated energy in order to prevent elastic unloading, and reads

$$c(\kappa, \alpha; \kappa_n, \alpha_n, \Delta s) := D(\kappa_n, \alpha_n, \kappa, \alpha) - \Delta s = 0. \quad (20)$$

This constraint is used in the dissipative parts of the equilibrium path. In case plastic effects are not present in the internal potential energy density (1), that is, in the case of brittle fracture, energy balance (9) and the weak form of the mechanical

balance equation (15a) can be used to rewrite this constraint in terms of the load multiplier and the displacement field only, recovering the dissipation-based path-following constraint of Gutiérrez²⁵:

$$c(\mathbf{u}, \lambda; \mathbf{u}_n, \lambda_n, \Delta s) = \frac{1}{2} \int_{\Gamma_N} \int_{t_n}^{t_{n+1}} \lambda \dot{\mathbf{t}} \cdot \dot{\mathbf{u}} \, d\tau \, dS - \frac{1}{2} \int_{\Gamma_N} \int_{t_n}^{t_{n+1}} \lambda \dot{\mathbf{t}} \cdot \mathbf{u} \, d\tau \, dS - \Delta s = 0. \quad (21)$$

Hereafter, the switch to the dissipation-based path-following constraint is performed after a fixed number of displacement control steps. The reader is referred to Verhoosel et al.²⁶ or May et al.³³ for automatic switching criteria based on a threshold of the dissipated energy. In addition, a constant and sufficiently small step size is considered in each example such that the proposed method converges for all time steps. Alternatively, adaptive step size techniques^{23,25,35} can be adopted.

2.4 | Spatial discretization and system matrices

The governing equations in weak form (17) are spatially discretized using finite elements with n_{node} nodes and n_{DOF} degrees of freedom, resulting in the following discrete system of non-linear equations in the load multiplier λ , the nodal quantities $\mathbf{u} \in \mathbb{R}^{n_{\text{DOF}}}$ and $\boldsymbol{\kappa}, \boldsymbol{\alpha}, \lambda_{\kappa}, \lambda_{\alpha_1}, \lambda_{\alpha_2} \in \mathbb{R}^{n_{\text{node}}}$:

$$\begin{cases} \mathbf{r}_u := \int_{\Omega} \mathbf{B}_v^T ((1 - \mathbf{N}_s \boldsymbol{\alpha})^2 \mathbf{C}^+ + \mathbf{C}^-) (\mathbf{B}_v \mathbf{u} - \boldsymbol{\epsilon}^p) \, d\mathbf{x} - \lambda \int_{\Gamma_N} \mathbf{N}_v^T \bar{\mathbf{t}} \, dS = \mathbf{0}, \\ \mathbf{r}_{\kappa} := \int_{\Omega} \mathbf{N}_s^T \left(-\sqrt{\frac{3}{2}} \|\boldsymbol{\sigma}_{\text{dev}}^{\text{tr}}\| + (1 - \mathbf{N}_s \boldsymbol{\alpha})^2 (\sigma^p + 3G \mathbf{N}_s (\boldsymbol{\kappa} - \boldsymbol{\kappa}_n)) - \mathbf{N}_s \lambda_{\kappa} \right) \, d\mathbf{x} = \mathbf{0}, \\ \mathbf{r}_{\alpha} := \int_{\Omega} \left[\mathbf{N}_s^T \left(-2(1 - \mathbf{N}_s \boldsymbol{\alpha}) (\psi^{e+} + \sigma^p \mathbf{N}_s \boldsymbol{\kappa}) + w'(\mathbf{N}_s \boldsymbol{\alpha}) - \mathbf{N}_s (\lambda_{\alpha_1} - \lambda_{\alpha_2}) \right) + \mathbf{B}_s^T \eta_d^2 \mathbf{B}_s \boldsymbol{\alpha} \right] \, d\mathbf{x} = \mathbf{0}. \end{cases} \quad (22)$$

In equation (22), $\mathbf{N}_s \in \mathbb{R}^{1 \times n_{\text{node}}}$ and $\mathbf{N}_v \in \mathbb{R}^{3 \times n_{\text{DOF}}}$ are the shape function matrices, and $\mathbf{B}_s \in \mathbb{R}^{3 \times n_{\text{node}}}$ and $\mathbf{B}_v \in \mathbb{R}^{6 \times n_{\text{DOF}}}$ are the discrete scalar and vector differential operators, respectively. Moreover, $\psi^{e+} := \frac{1}{2} \|\mathbf{B}_v \mathbf{u} - \boldsymbol{\epsilon}^p\|_{\mathbf{C}^+}^2 \in \mathbb{R}_+$ denotes the discrete degradable part of the elastic energy density, where, in Voigt notation, $\boldsymbol{\epsilon}^p := \boldsymbol{\epsilon}_n^p + \sqrt{3/2} \hat{\mathbf{n}}^{\text{tr}} \mathbf{N}_s (\boldsymbol{\kappa} - \boldsymbol{\kappa}_n) \in \mathbb{R}^6$ is the plastic strain vector, $\boldsymbol{\sigma}_{\text{dev}}^{\text{tr}} \in \mathbb{R}^6$ is the deviatoric part of the trial stress, $\hat{\mathbf{n}}^{\text{tr}} \in \mathbb{R}^6$ is the direction of the plastic flow at the trial state, and $\mathbf{C}^+ \in \mathbb{R}_{\text{sym}}^{6 \times 6}$ and $\mathbf{C}^- \in \mathbb{R}_{\text{sym}}^{6 \times 6}$ are the constitutive matrices corresponding to the decomposition of the elastic energy density in equation (2). The function $w'(\mathbf{N}_s \boldsymbol{\alpha})$ equals w_0 for the AT-1 model and $2w_0 \mathbf{N}_s \boldsymbol{\alpha}$ for the AT-2 model. The Jacobian matrices $\mathbf{K}_{\square \bullet} := \frac{\partial \mathbf{r}_{\square}}{\partial \bullet}$ of the system in (22) read

$$\begin{aligned} \mathbf{K}_{uu} &= \int_{\Omega} \mathbf{B}_v^T ((1 - \mathbf{N}_s \boldsymbol{\alpha})^2 \mathbf{C}^+ + \mathbf{C}^-) \mathbf{B}_v \, d\mathbf{x}, \\ \mathbf{K}_{\kappa \kappa} &= \int_{\Omega} 3G (1 - \mathbf{N}_s \boldsymbol{\alpha})^2 \mathbf{N}_s^T \mathbf{N}_s \, d\mathbf{x}, \\ \mathbf{K}_{\alpha \alpha} &= \int_{\Omega} \left[\mathbf{N}_s^T \mathbf{N}_s \left(2\psi^{e+} + 2\sigma^p \mathbf{N}_s \boldsymbol{\kappa} + w''(\mathbf{N}_s \boldsymbol{\alpha}) \right) + \mathbf{B}_s^T \eta_d^2 \mathbf{B}_s \right] \, d\mathbf{x}, \\ \mathbf{K}_{u\kappa} &= \mathbf{K}_{\kappa u}^T = \int_{\Omega} -\sqrt{\frac{3}{2}} \mathbf{B}_v^T ((1 - \mathbf{N}_s \boldsymbol{\alpha})^2 \mathbf{C}^+ + \mathbf{C}^-) \hat{\mathbf{n}}^{\text{tr}} \mathbf{N}_s \, d\mathbf{x}, \\ \mathbf{K}_{u\alpha} &= \mathbf{K}_{\alpha u}^T = \int_{\Omega} -2(1 - \mathbf{N}_s \boldsymbol{\alpha}) \mathbf{B}_v^T \mathbf{C}^+ (\mathbf{B}_v \mathbf{u} - \boldsymbol{\epsilon}^p) \mathbf{N}_s \, d\mathbf{x}, \\ \mathbf{K}_{u\lambda} &= -\mathbf{P} = -\int_{\Gamma_N} \mathbf{N}_v^T \bar{\mathbf{t}} \, dS, \\ \mathbf{K}_{\kappa \alpha} &= \mathbf{K}_{\alpha \kappa}^T = \int_{\Omega} -2(1 - \mathbf{N}_s \boldsymbol{\alpha}) \mathbf{N}_s^T \mathbf{N}_s \left(-\sqrt{\frac{3}{2}} (\mathbf{B}_v \mathbf{u} - \boldsymbol{\epsilon}^p)^T \mathbf{C}^+ \hat{\mathbf{n}}^{\text{tr}} + \sigma^p \right) \, d\mathbf{x}, \\ \mathbf{K}_{\kappa \lambda_{\kappa}} &= \mathbf{K}_{\alpha \lambda_{\alpha_1}} = -\mathbf{K}_{\alpha \lambda_{\alpha_2}} = \int_{\Omega} -\mathbf{N}_s^T \mathbf{N}_s \, d\mathbf{x}, \end{aligned} \quad (23)$$

where the direction of the plastic flow is considered to be independent of the displacement field, and the function $w''(\mathbf{N}_s \boldsymbol{\alpha})$ equals zero if the AT-1 model is used and $2w_0$ if the AT-2 model is used. In addition, the KKT conditions (18) are discretized as

$$\begin{cases} \mathbf{r}_{\lambda_\kappa} := \boldsymbol{\Lambda}_\kappa (\boldsymbol{\kappa} - \boldsymbol{\kappa}_n) = \mathbf{0}, & \lambda_\kappa \geq 0, & (\boldsymbol{\kappa} - \boldsymbol{\kappa}_n) \geq \mathbf{0}, \\ \mathbf{r}_{\lambda_{\alpha_1}} := \boldsymbol{\Lambda}_{\alpha_1} (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) = \mathbf{0}, & \lambda_{\alpha_1} \geq 0, & (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) \geq \mathbf{0}, \\ \mathbf{r}_{\lambda_{\alpha_2}} := \boldsymbol{\Lambda}_{\alpha_2} (\mathbf{e} - \boldsymbol{\alpha}) = \mathbf{0}, & \lambda_{\alpha_2} \geq 0, & (\mathbf{e} - \boldsymbol{\alpha}) \geq \mathbf{0}, \end{cases} \quad (24)$$

where $\mathbf{e} \in \mathbb{R}^{n_{\text{node}}}$ is a vector of ones, and $\boldsymbol{\Lambda}_\kappa, \boldsymbol{\Lambda}_{\alpha_1}, \boldsymbol{\Lambda}_{\alpha_2} \in \mathbb{R}^{n_{\text{node}} \times n_{\text{node}}}$ are diagonal matrices, whose diagonal entries are given by the components of $\lambda_\kappa, \lambda_{\alpha_1}$, and λ_{α_2} , respectively.

The displacement control path-following constraint (19) is discretized as

$$\mathbf{r}_\lambda := \mathbf{L}(\mathbf{u} - \mathbf{u}_n) - \Delta s = 0, \quad (25)$$

where $\mathbf{L} \in \mathbb{R}^{1 \times n_{\text{DOF}}}$ is a selection matrix that selects the controlled displacement from $\mathbf{u}$. The Jacobian matrices read

$$\mathbf{K}_{\lambda u} = \mathbf{L}, \quad \mathbf{K}_{\lambda \lambda} = 0, \quad \mathbf{K}_{\lambda \kappa} = \mathbf{0}, \quad \text{and} \quad \mathbf{K}_{\lambda \alpha} = \mathbf{0}. \quad (26)$$

The dissipation-based path-following constraints (20) and (21) are discretized as

$$\begin{aligned} \mathbf{r}_\lambda := \int_{\Omega} \left[\left((1 - \mathbf{N}_s \boldsymbol{\alpha})^2 \sigma^p \mathbf{N}_s \boldsymbol{\kappa} + w(\mathbf{N}_s \boldsymbol{\alpha}) + \frac{1}{2} \eta_d^2 \|\mathbf{B}_s \boldsymbol{\alpha}\|^2 \right) \right. \\ \left. - \left((1 - \mathbf{N}_s \boldsymbol{\alpha}_n)^2 \sigma^p \mathbf{N}_s \boldsymbol{\kappa}_n + w(\mathbf{N}_s \boldsymbol{\alpha}_n) + \frac{1}{2} \eta_d^2 \|\mathbf{B}_s \boldsymbol{\alpha}_n\|^2 \right) \right] d\mathbf{x} - \Delta s = 0, \end{aligned} \quad (27)$$

and

$$\mathbf{r}_\lambda := \frac{1}{2} \lambda_n \int_{\Gamma_N} \bar{\mathbf{t}}^T \mathbf{N}_v (\mathbf{u} - \mathbf{u}_n) dS - \frac{1}{2} (\lambda - \lambda_n) \int_{\Gamma_N} \bar{\mathbf{t}}^T \mathbf{N}_v \mathbf{u}_n dS - \Delta s = 0, \quad (28)$$

respectively. The function $w(\mathbf{N}_s \boldsymbol{\alpha})$ equals $w_0 \mathbf{N}_s \boldsymbol{\alpha}$ for the AT-1 model and $w_0 (\mathbf{N}_s \boldsymbol{\alpha})^2$ for the AT-2 model. The Jacobian matrices of equations (27) and (28) read

$$\begin{aligned} \mathbf{K}_{\lambda u} = \mathbf{0}, \quad \mathbf{K}_{\lambda \lambda} = 0, \quad \mathbf{K}_{\lambda \kappa} = \int_{\Omega} (1 - \mathbf{N}_s \boldsymbol{\alpha})^2 \sigma^p \mathbf{N}_s d\mathbf{x}, \\ \mathbf{K}_{\lambda \alpha} = \int_{\Omega} \left(-2(1 - \mathbf{N}_s \boldsymbol{\alpha}) \sigma^p \mathbf{N}_s \boldsymbol{\kappa} \mathbf{N}_s + w'(\mathbf{N}_s \boldsymbol{\alpha}) \mathbf{N}_s + \boldsymbol{\alpha}^T \mathbf{B}_s^T \eta_d^2 \mathbf{B}_s \right) d\mathbf{x}, \end{aligned} \quad (29)$$

and

$$\mathbf{K}_{\lambda u} = \frac{1}{2} \lambda_n \int_{\Gamma_N} \bar{\mathbf{t}}^T \mathbf{N}_v dS, \quad \mathbf{K}_{\lambda \lambda} = -\frac{1}{2} \int_{\Gamma_N} \bar{\mathbf{t}}^T \mathbf{N}_v \mathbf{u}_n dS, \quad \mathbf{K}_{\lambda \kappa} = \mathbf{0}, \quad \mathbf{K}_{\lambda \alpha} = \mathbf{0}, \quad (30)$$

respectively.

The system of equations (22), the KKT conditions (24), and one of the discretized path-following constraints (25), (27) or (28) represent the set of equations from which the primal variables $\{\mathbf{u}, \lambda, \boldsymbol{\kappa}, \boldsymbol{\alpha}\}$ and the dual variables $\{\lambda_\kappa, \lambda_{\alpha_1}, \lambda_{\alpha_2}\}$ can be computed. The next section presents an algorithm based on interior-point methods for the monolithic solution of this constrained system of equations.

3 | DISSIPATION-BASED MONOLITHIC SCHEME

This section presents an algorithm for the monolithic solution of the constrained system of equations (22) and (24) augmented by a path-following constraint. An interior-point method is used to rigorously impose the constraints on the equivalent plastic strain and the crack phase-field. First, a perturbation is applied to the KKT conditions, and a sequence of perturbations is considered, which recovers the original KKT conditions (24) in the limit. Second, the augmented primal-dual system is obtained through linearization. A partitioned procedure is proposed, allowing to efficiently compute the undamped Newton step. Finally, a damped Newton step is computed, considering the inequality constraints in the KKT conditions.

Two techniques which allow imposing dissipation in either tension or compression are presented. Augmenting the equations by a dissipation-based path-following constraint allows tracing the equilibrium path without time-discontinuous jumps. As such, it

is expected that the monolithic scheme is more robust provided that the step sizes are sufficiently small. In this paper, convergence is achieved if the infinity norm of the residuals in (22) and (24) augmented by a path-following constraint is smaller than a user-defined tolerance TOL, i.e. $\max\{\|\mathbf{r}_u\|_\infty, \|\mathbf{r}_\kappa\|_\infty, \|\mathbf{r}_\alpha\|_\infty, |r_\lambda|, \|\mathbf{r}_{\lambda_\kappa}\|_\infty, \|\mathbf{r}_{\lambda_{\alpha_1}}\|_\infty, \|\mathbf{r}_{\lambda_{\alpha_2}}\|_\infty\} \leq \text{TOL}$. Alternatively, different tolerances for each residual or relative tolerances can be used. However, for simplicity, a single tolerance in combination with an absolute convergence criterion is adopted hereafter.

Perturbation of the KKT conditions

The following perturbation is applied to the KKT conditions:

$$\begin{cases} \mathbf{r}_{\lambda_\kappa} \approx \Lambda_\kappa(\boldsymbol{\kappa} - \boldsymbol{\kappa}_n) - \mu^{(k)} \mathbf{e} = \mathbf{0}, & \lambda_\kappa \geq 0, & (\boldsymbol{\kappa} - \boldsymbol{\kappa}_n) \geq \mathbf{0}, \\ \mathbf{r}_{\lambda_{\alpha_1}} \approx \Lambda_{\alpha_1}(\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) - \mu^{(k)} \mathbf{e} = \mathbf{0}, & \lambda_{\alpha_1} \geq 0, & (\boldsymbol{\alpha} - \boldsymbol{\alpha}_n) \geq \mathbf{0}, \\ \mathbf{r}_{\lambda_{\alpha_2}} \approx \Lambda_{\alpha_2}(\mathbf{e} - \boldsymbol{\alpha}) - \mu^{(k)} \mathbf{e} = \mathbf{0}, & \lambda_{\alpha_2} \geq 0, & (\mathbf{e} - \boldsymbol{\alpha}) \geq \mathbf{0}, \end{cases} \quad (31)$$

where $\mu^{(k)} \in \mathbb{R}_+$ is the barrier parameter. This perturbation can be obtained by approximating the indicator functions $I_{[\kappa_n, +\infty)}(\kappa)$ and $I_{[\alpha_n, 1]}(\alpha)$ by the smooth log-barrier terms $-\mu^{(k)} \log(\kappa - \kappa_n)$, $-\mu^{(k)} \log(\alpha - \alpha_n)$ and $-\mu^{(k)} \log(1 - \alpha)$ (see e.g. Nocedal and Wright⁴⁸). The perturbed problem is solved for a sequence of barrier parameters $\{\mu^{(k)}\}$ that converges to zero, with $k \in \mathbb{N} \cup \{0\}$. Only one iteration is performed for a given barrier parameter, as commonly done with interior-point methods⁴⁸. As such, the counter k of the sequence of barrier parameters $\{\mu^{(k)}\}$ coincides with the iteration counter of the approximated primal variables $\{\mathbf{u}^{(k)}, \lambda^{(k)}, \boldsymbol{\kappa}^{(k)}, \boldsymbol{\alpha}^{(k)}\}$ and dual variables $\{\lambda_\kappa^{(k)}, \lambda_{\alpha_1}^{(k)}, \lambda_{\alpha_2}^{(k)}\}$. After each iteration, the barrier parameter is updated, and the linearization is repeated.

Augmented primal-dual system

Linearization of equations (22) and (31) augmented by one of the discretized path-following constraints (25), (27) or (28) leads to the following augmented primal-dual system:

$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\kappa} & \mathbf{K}_{u\alpha} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{P} \\ \mathbf{K}_{\kappa u} & \mathbf{K}_{\kappa\kappa} & \mathbf{K}_{\kappa\alpha} & \mathbf{K}_{\kappa\lambda_\kappa} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{\alpha u} & \mathbf{K}_{\alpha\kappa} & \mathbf{K}_{\alpha\alpha} & \mathbf{0} & \mathbf{K}_{\alpha\lambda_{\alpha_1}} & \mathbf{K}_{\alpha\lambda_{\alpha_2}} & \mathbf{0} \\ \mathbf{0} & \Lambda_\kappa & \mathbf{0} & \mathbf{S}_\kappa & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \Lambda_{\alpha_1} & \mathbf{0} & \mathbf{S}_{\alpha_1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\Lambda_{\alpha_2} & \mathbf{0} & \mathbf{0} & \mathbf{S}_{\alpha_2} & \mathbf{0} \\ \mathbf{K}_{\lambda u} & \mathbf{K}_{\lambda\kappa} & \mathbf{K}_{\lambda\alpha} & \mathbf{0} & \mathbf{0} & \mathbf{0} & K_{\lambda\lambda} \end{bmatrix}^{(k)} \begin{bmatrix} \Delta \mathbf{u} \\ \Delta \boldsymbol{\kappa} \\ \Delta \boldsymbol{\alpha} \\ \Delta \lambda_\kappa \\ \Delta \lambda_{\alpha_1} \\ \Delta \lambda_{\alpha_2} \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \mathbf{r}_u \\ \mathbf{r}_\kappa \\ \mathbf{r}_\alpha \\ \mathbf{r}_{\lambda_\kappa} \\ \mathbf{r}_{\lambda_{\alpha_1}} \\ \mathbf{r}_{\lambda_{\alpha_2}} \\ r_\lambda \end{bmatrix}^{(k)}, \quad (32)$$

where $\mathbf{S}_\kappa, \mathbf{S}_{\alpha_1}, \mathbf{S}_{\alpha_2} \in \mathbb{R}^{n_{\text{node}} \times n_{\text{node}}}$ are diagonal matrices whose diagonal entries are given by the components of the inequality constraints $\boldsymbol{\kappa}^{(k)} - \boldsymbol{\kappa}_n$, $\boldsymbol{\alpha}^{(k)} - \boldsymbol{\alpha}_n$, and $\mathbf{e} - \boldsymbol{\alpha}^{(k)}$, respectively. The augmented primal-dual system can be condensed by eliminating the dual variables, resulting in the following reduced primal-dual system:

$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\kappa} & \mathbf{K}_{u\alpha} & -\mathbf{P} \\ \mathbf{K}_{\kappa u} & \mathbf{K}'_{\kappa\kappa} & \mathbf{K}'_{\kappa\alpha} & \mathbf{0} \\ \mathbf{K}_{\alpha u} & \mathbf{K}_{\alpha\kappa} & \mathbf{K}'_{\alpha\alpha} & \mathbf{0} \\ \mathbf{K}_{\lambda u} & \mathbf{K}_{\lambda\kappa} & \mathbf{K}_{\lambda\alpha} & K_{\lambda\lambda} \end{bmatrix}^{(k)} \begin{bmatrix} \Delta \mathbf{u} \\ \Delta \boldsymbol{\kappa} \\ \Delta \boldsymbol{\alpha} \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \mathbf{r}_u \\ \mathbf{r}'_\kappa \\ \mathbf{r}'_\alpha \\ r_\lambda \end{bmatrix}^{(k)}, \quad (33)$$

with

$$\begin{aligned} \mathbf{K}'_{\kappa\kappa} &:= \mathbf{K}_{\kappa\kappa}^{(k)} - \mathbf{K}_{\kappa\lambda_\kappa}^{(k)} \Lambda_\kappa^{(k)} \mathbf{S}_\kappa^{-1}, \\ \mathbf{r}'_\kappa &:= \mathbf{r}_\kappa^{(k)} - \mathbf{K}_{\kappa\lambda_\kappa}^{(k)} (\lambda_\kappa^{(k)} - \mu^{(k)} \mathbf{S}_\kappa^{-1} \mathbf{e}), \\ \mathbf{K}'_{\alpha\alpha} &:= \mathbf{K}_{\alpha\alpha}^{(k)} - \mathbf{K}_{\alpha\lambda_{\alpha_1}}^{(k)} \Lambda_{\alpha_1}^{(k)} \mathbf{S}_{\alpha_1}^{-1} + \mathbf{K}_{\alpha\lambda_{\alpha_2}}^{(k)} \Lambda_{\alpha_2}^{(k)} \mathbf{S}_{\alpha_2}^{-1}, \\ \mathbf{r}'_\alpha &:= \mathbf{r}_\alpha^{(k)} - \mathbf{K}_{\alpha\lambda_{\alpha_1}}^{(k)} (\lambda_{\alpha_1}^{(k)} - \mu^{(k)} \mathbf{S}_{\alpha_1}^{-1} \mathbf{e}) - \mathbf{K}_{\alpha\lambda_{\alpha_2}}^{(k)} (\lambda_{\alpha_2}^{(k)} - \mu^{(k)} \mathbf{S}_{\alpha_2}^{-1} \mathbf{e}). \end{aligned} \quad (34)$$

The step of the dual variables is then obtained as follows:

$$\begin{aligned}\Delta\lambda_\kappa &= -\lambda_\kappa^{(k)} - \mathbf{S}_\kappa^{-1}(\Lambda_\kappa^{(k)}\Delta\boldsymbol{\kappa} - \mu^{(k)}\mathbf{e}), \\ \Delta\lambda_{\alpha_1} &= -\lambda_{\alpha_1}^{(k)} - \mathbf{S}_{\alpha_1}^{-1}(\Lambda_{\alpha_1}^{(k)}\Delta\boldsymbol{\alpha} - \mu^{(k)}\mathbf{e}), \\ \Delta\lambda_{\alpha_2} &= -\lambda_{\alpha_2}^{(k)} - \mathbf{S}_{\alpha_2}^{-1}(-\Lambda_{\alpha_2}^{(k)}\Delta\boldsymbol{\alpha} - \mu^{(k)}\mathbf{e}),\end{aligned}\quad (35)$$

which can be easily computed, owing to the diagonal structure of $\mathbf{S}_\kappa$, $\mathbf{S}_{\alpha_1}$, and $\mathbf{S}_{\alpha_2}$.

A selective integration rule is used, where the terms involving the dual variables are integrated using quadrature points that coincide with the nodes. As such, $\mathbf{K}_{\kappa\lambda_\kappa}$, $\mathbf{K}_{\alpha\lambda_{\alpha_1}}$ and $\mathbf{K}_{\alpha\lambda_{\alpha_2}}$ become diagonal and $\mathbf{K}'_{\kappa\kappa}$ and $\mathbf{K}'_{\alpha\alpha}$ become symmetric. However, due to the auxiliary path-following constraint, the system matrix in equation (33) is unsymmetric. Therefore, the linear system is solved using a partitioned procedure:

$$\begin{cases} \Delta\lambda = \frac{[\mathbf{K}_{\lambda u} \ \mathbf{K}_{\lambda\kappa} \ \mathbf{K}_{\lambda\alpha}]^{(k)} \mathbf{v}_I - \mathbf{r}_\lambda^{(k)}}{\mathbf{K}'_{\lambda\lambda}^{(k)} - [\mathbf{K}_{\lambda u} \ \mathbf{K}_{\lambda\kappa} \ \mathbf{K}_{\lambda\alpha}]^{(k)} \mathbf{v}_{II}}, \\ [\Delta\mathbf{u}^T \ \Delta\boldsymbol{\kappa}^T \ \Delta\boldsymbol{\alpha}^T]^T = -\mathbf{v}_I - \Delta\lambda \mathbf{v}_{II}, \end{cases}\quad (36)$$

where $\mathbf{v}_I \in \mathbb{R}^{n_{\text{DOF}}+2n_{\text{node}}}$ and $\mathbf{v}_{II} \in \mathbb{R}^{n_{\text{DOF}}+2n_{\text{node}}}$ are the solutions of $\mathbf{K}'\mathbf{v}_I = \mathbf{r}_I$ and $\mathbf{K}'\mathbf{v}_{II} = \mathbf{r}_{II}$, respectively, with

$$\mathbf{K}' := \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\kappa} & \mathbf{K}_{u\alpha} \\ \mathbf{K}_{\kappa u} & \mathbf{K}'_{\kappa\kappa} & \mathbf{K}_{\kappa\alpha} \\ \mathbf{K}_{\alpha u} & \mathbf{K}_{\alpha\kappa} & \mathbf{K}'_{\alpha\alpha} \end{bmatrix}^{(k)}, \quad \mathbf{r}_I := \begin{bmatrix} \mathbf{r}_u \\ \mathbf{r}_\kappa \\ \mathbf{r}_\alpha \end{bmatrix}^{(k)}, \quad \text{and} \quad \mathbf{r}_{II} := \begin{bmatrix} -\mathbf{P} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad (37)$$

where the $\mathbf{K}'$ is symmetric as a result of the selective integration rule for $\mathbf{K}_{\kappa\lambda_\kappa}$, $\mathbf{K}_{\alpha\lambda_{\alpha_1}}$ and $\mathbf{K}_{\alpha\lambda_{\alpha_2}}$. As such, the partitioned procedure involves solving two symmetric systems with a system matrix $\mathbf{K}'$ and two different right-hand sides $\mathbf{r}_I \in \mathbb{R}^{n_{\text{DOF}}+2n_{\text{node}}}$ and $\mathbf{r}_{II} \in \mathbb{R}^{n_{\text{DOF}}+2n_{\text{node}}}$. Provided that $\mathbf{K}'$ is non-singular, this computation can be performed efficiently to obtain both $\mathbf{v}_I$ and $\mathbf{v}_{II}$ using one factorization of $\mathbf{K}'$. Since $\mathbf{K}'$ can be indefinite, the MA57 routine in the Harwell Subroutine Library⁴⁹ is used for its symmetric indefinite factorization. Alternatively, when $\mathbf{K}'$ is positive definite, a Cholesky factorization is performed using CHOLMOD⁵⁰.

Damped Newton step

A damped Newton step is performed with step lengths $t^{\text{prim}} \in \mathbb{R}_+$ and $t^{\text{dual}} \in \mathbb{R}_+$ such that the inequality constraints in the KKT conditions (31) hold for all iterations. The step lengths are computed as

$$\begin{aligned} t^{\text{prim}} &:= \max \left\{ t \in (0, 1] \mid \begin{bmatrix} \boldsymbol{\kappa}^{(k)} - \boldsymbol{\kappa}_n \\ \boldsymbol{\alpha}^{(k)} - \boldsymbol{\alpha}_n \\ \mathbf{e} - \boldsymbol{\alpha}^{(k)} \end{bmatrix} + t \begin{bmatrix} \Delta\boldsymbol{\kappa} \\ \Delta\boldsymbol{\alpha} \\ -\Delta\boldsymbol{\alpha} \end{bmatrix} \geq (1 - \tau) \begin{bmatrix} \boldsymbol{\kappa}^{(k)} - \boldsymbol{\kappa}_n \\ \boldsymbol{\alpha}^{(k)} - \boldsymbol{\alpha}_n \\ \mathbf{e} - \boldsymbol{\alpha}^{(k)} \end{bmatrix} \right\}, \\ t^{\text{dual}} &:= \max \left\{ t \in (0, 1] \mid \begin{bmatrix} \lambda_\kappa^{(k)} \\ \lambda_{\alpha_1}^{(k)} \\ \lambda_{\alpha_2}^{(k)} \end{bmatrix} + t \begin{bmatrix} \Delta\lambda_\kappa \\ \Delta\lambda_{\alpha_1} \\ \Delta\lambda_{\alpha_2} \end{bmatrix} \geq (1 - \tau) \begin{bmatrix} \lambda_\kappa^{(k)} \\ \lambda_{\alpha_1}^{(k)} \\ \lambda_{\alpha_2}^{(k)} \end{bmatrix} \right\}, \end{aligned}\quad (38)$$

where $\tau \in (0, 1)$ is a constant which prevents the inequality constraints and the dual variables from approaching their lower bound of zero too quickly⁴⁸. A too small value of τ prevents the algorithm from taking large steps, while a too large value of τ allows steps that are too close to the lower bounds of the constrained fields. Hereinafter, a value of 0.999 is assigned to τ . The values of the new iterate are then given by

$$\begin{aligned} \{\mathbf{u}^{(k+1)}, \lambda^{(k+1)}, \boldsymbol{\kappa}^{(k+1)}, \boldsymbol{\alpha}^{(k+1)}\} &:= \{\mathbf{u}^{(k)}, \lambda^{(k)}, \boldsymbol{\kappa}^{(k)}, \boldsymbol{\alpha}^{(k)}\} + t^{\text{prim}} \{\Delta\mathbf{u}, \Delta\lambda, \Delta\boldsymbol{\kappa}, \Delta\boldsymbol{\alpha}\}, \\ \{\lambda_\kappa^{(k+1)}, \lambda_{\alpha_1}^{(k+1)}, \lambda_{\alpha_2}^{(k+1)}\} &:= \{\lambda_\kappa^{(k)}, \lambda_{\alpha_1}^{(k)}, \lambda_{\alpha_2}^{(k)}\} + t^{\text{dual}} \{\Delta\lambda_\kappa, \Delta\lambda_{\alpha_1}, \Delta\lambda_{\alpha_2}\}. \end{aligned}\quad (39)$$

Avoiding load-reversals

The dissipation potential (5) does not distinguish between dissipation in tension or compression. As such, controlling the dissipated energy is not sufficient to obtain a response in either tension or compression with a positive load multiplier. Therefore, two novel techniques are presented that avoid a negative load multiplier.

The first technique can only be applied in a one-dimensional setting, and modifies the incremental equations (17) to a Rankine criterion combined with a tension-compression split:

$$\begin{cases} \int_{\Omega} \sigma(\epsilon, \epsilon^p(\kappa), \alpha) \tilde{u}' d\mathbf{x} - \lambda \int_{\Gamma_N} \tilde{t} \tilde{u} dS = 0, \\ \int_{\Omega} \left(-\sigma^{\text{tr}}(\epsilon, \alpha; \epsilon_n^p) + g(\alpha)(\sigma^p + E(\kappa - \kappa_n)) - \lambda_{\kappa} \right) |\tilde{\epsilon}^p| d\mathbf{x} = 0, \\ \int_{\Omega} \left[\left(g'(\alpha)(\psi^{\epsilon+}(\epsilon, \epsilon^p(\kappa)) + \sigma^p \kappa) + w'(\alpha) - (\lambda_{\alpha_1} - \lambda_{\alpha_2}) \right) \tilde{\alpha} + \eta_d^2 \alpha' \tilde{\alpha}' \right] d\mathbf{x} = 0, \end{cases} \quad (40)$$

where E is the Young's modulus, and $\tilde{u}'$, α' and $\tilde{\alpha}'$ are the spatial derivatives along the one-dimensional axis of $\tilde{u}$, α and $\tilde{\alpha}$, respectively. As such, dissipation occurs in either tension or compression and, when the dissipated energy is controlled, a response with a positive load multiplier is obtained.

The second technique is more general and renders the load multiplier positive during all iterations of a given time step by replacing the step size t^{prim} in equation (38) with

$$\tilde{t}^{\text{prim}} := \max \{ t \in (0, t^{\text{prim}}] \mid \lambda^{(k)} + t \Delta \lambda \geq (1 - \tau) \lambda^{(k)} \}. \quad (41)$$

As such, the step size $\tilde{t}^{\text{prim}} \leq t^{\text{prim}}$ is decreased, and it is ensured that the load multiplier is strictly positive during all iterations. In order to limit possible adverse effects of this reduction, the computations are first performed using the step size t^{prim} in equation (38). If the algorithm converges to a negative load multiplier, the time step is recomputed using the step size $\tilde{t}^{\text{prim}}$ in equation (41).

Computation of the barrier parameter

In the limit, the sequence of barrier parameters $\{\mu^{(k)}\}$ must converge to zero, in order to recover the original KKT conditions (24). An adaptive strategy based on a predictor direction is employed⁴⁸. This heuristic technique requires solving the primal-dual system (33) and (35) with $\mu^{(k)} = 0$ to obtain the affine-scaling direction $\{\Delta \kappa^{\text{aff}}, \Delta \alpha^{\text{aff}}, \Delta \lambda_{\kappa}^{\text{aff}}, \Delta \lambda_{\alpha_1}^{\text{aff}}, \Delta \lambda_{\alpha_2}^{\text{aff}}\}$. The barrier parameter is then computed as

$$\mu^{(k)} := \frac{\left[(\kappa^{\text{aff}} - \kappa_n)^T \lambda_{\kappa}^{\text{aff}} + (\alpha^{\text{aff}} - \alpha_n)^T \lambda_{\alpha_1}^{\text{aff}} + (\mathbf{e} - \alpha^{\text{aff}})^T \lambda_{\alpha_2}^{\text{aff}} \right]^3}{n_{\text{const}} \left[(\kappa^{(k)} - \kappa_n)^T \lambda_{\kappa}^{(k)} + (\alpha^{(k)} - \alpha_n)^T \lambda_{\alpha_1}^{(k)} + (\mathbf{e} - \alpha^{(k)})^T \lambda_{\alpha_2}^{(k)} \right]^2}, \quad (42)$$

where n_{const} is the total number of nodal constraints, and κ^{aff} , α^{aff} , $\lambda_{\kappa}^{\text{aff}}$, $\lambda_{\alpha_1}^{\text{aff}}$ and $\lambda_{\alpha_2}^{\text{aff}}$ are computed with equations (38), (39) and (41) using the affine-scaling direction.

Starting values

First, it is checked if any damage value of the previous time step exceeds a threshold CRTOL. If so, those damage variables are fixed to 1 in the current time step, and the corresponding monotonicity and upper bound constraints are removed from the primal-dual system. Hereafter, a value of 0.999 is assigned to CRTOL. Second, the internal variables which are not fixed are initialized at the values of the previous time step plus a small increment, such that all inequalities hold strictly (e.g. $\alpha^{(0)} := \alpha_n + (1 - \text{CRTOL})\mathbf{e}$ and $\kappa^{(0)} := \kappa_n + (1 - \text{CRTOL})\mathbf{e}$). As such, the approximations of the inequality-constrained variables stay in the feasible domain, as is commonly the case for interior-point methods⁴⁸. Third, the load multiplier is initialized at the value of the previous time step (i.e. $\lambda^{(0)} := \lambda_n$). Fourth, the initial estimate $\mathbf{u}^{(0)}$ of the displacement field is computed by freezing all the internal variables and taking an elastic step (i.e. solving the first equation in (22) for fixed internal variables). Finally, the dual variables are initialized using the heuristic approach proposed in Gertz et al.⁵¹ by computing the affine-scaling direction $\{\Delta \lambda_{\kappa}^{\text{aff}(0)}, \Delta \lambda_{\alpha_1}^{\text{aff}(0)}, \Delta \lambda_{\alpha_2}^{\text{aff}(0)}\}$ and computing each component $\lambda^{(0)} \in \{\lambda_{\kappa}^{(0)}, \lambda_{\alpha_1}^{(0)}, \lambda_{\alpha_2}^{(0)}\}$ as $\max\{1, |1 + \Delta \lambda^{\text{aff}(0)}|\}$.

4 | NUMERICAL EXAMPLES

This section illustrates the performance of the presented method using four numerical examples. The first example considers brittle fracture in a two-dimensional setting where a crack initiates at a notch and, when displacements are imposed, propagates brutally through the specimen. However, when a path-following technique is adopted, snap-backs can be observed. In the second example, the same specimen is loaded horizontally resulting in a crack that propagates less brutally through a region of high tensile stresses. This example shows a snap-back when the specimen is close to fracturing completely. The third example considers ductile fracture in a one-dimensional bar, where plastic strains first grow homogeneously followed by the localization of the plastic strains and the crack phase-field in the middle of the bar. A snap-back occurs when damage initiates, and the influence of the damage length scale is investigated. Finally, in the fourth example, ductile fracture is considered in a two-dimensional specimen, showing a similar behavior as the one-dimensional bar. In all examples, the element size h_c is chosen significantly smaller than the damage characteristic length ℓ_d .

The software used for the computations is an extension of *Stabil*⁵², an open-source MATLAB toolbox developed at the Structural Mechanics section of KU Leuven. The extension to fracture problems is implemented in MATLAB and C++. The C++ code is used to assemble all system matrices, and MATLAB is used to perform the computations of the presented monolithic scheme. All computations are performed on an Intel(R) Xeon(R) Gold 6140 2.30 GHz processor.

4.1 | Single-edge notched specimen subject to tension

The example of the single-edge notched specimen was originally proposed by Bourdin et al.⁵³, and was later adopted as a benchmark problem by many authors^{2,3,5,6,8–13,32,35,39}. In this example, a square specimen with sides of 1 mm and a pre-existing notch is considered (figure 1). The bottom edge remains completely fixed, while a vertical load is imposed on the top edge. In addition, constraint equations are used to constrain the top edge, such that all vertical displacements are the same. The specimen behaves in a brittle way, governed by an AT-2 model, and has a bulk modulus $K = 175000$ MPa, a shear modulus $G = 80769.23$ MPa, a local damage dissipation constant $w_0 = 135$ MPa and a damage length scale $\eta_d = 0.164$ N^{1/2}, corresponding to the material properties in Gerasimov and De Lorenzis¹¹, i.e. a fracture toughness $G_c = 2.7$ N/mm and a damage characteristic length $\ell_d = 0.01$ mm. In addition, plane strain conditions are assumed. A finite element discretization with 17234 bilinear quadrilateral elements and 17421 nodes is considered, corresponding to an element size $h_c = 0.0025$ mm in the critical zone where fracture is expected to occur. In addition, meshes with different element sizes have been considered, resulting in similar results which are not shown for brevity. For this example, a tolerance $TOL = 10^{-6}$ is used.

FIGURE 1 Geometry and boundary conditions of the single-edge notched specimen subject to tension. The dimensions are given in mm.

Figure 2(a) shows the equilibrium path for the single-edge notched specimen subject to tension obtained by imposing displacements on the top edge in 50 steps of 10^{-4} mm, followed by controlling the dissipated energy in steps of 5×10^{-7} J. The displacement and dissipated energy are imposed using the displacement control path-following constraint (19) and dissipation-based path-following constraint (21), respectively. Because the specimen is brittle and plastic effects are not present, the dissipation can be expressed in terms of the displacement field and the load multiplier. For all time steps, the proposed method converges to a response with a positive load multiplier without requiring any modifications of the step size t^{prim} according to equation (41). On average, the proposed method requires 16.5 iterations per time step, corresponding to a computational time of 21.6 s per time step.

FIGURE 2 (a) Equilibrium path and (b) energy evolution for the single-edge notched specimen subject to tension. The markers correspond to the time steps at which the crack phase-field is shown in figure 3.

In the first stage of the loading process, the specimen behaves quasi-linearly and shows a slow damage evolution as a consequence of the AT-2 model. When the displacement control path-following constraint (19) is used throughout the entire loading history (i.e. between 0 mm and 6×10^{-3} mm), convergence cannot be obtained after the peak load is reached. At this time step, the equilibrium path shows a time-discontinuous jump and the snap-back is not captured. Alternatively, when a dissipation-based path-following technique is adopted, this jump does not occur and the presented method converges. During the nucleation of the crack phase-field at the end of the notch, a snap-back occurs. This snap-back is not observed in case the tip of the notch is enriched by a phase-field function, or when the notch is modeled using initial damage values (see e.g. Singh et al.³⁵). Once the phase-field has nucleated, the force drops without a significant change in the vertical displacements, and a snap-back occurs when the specimen fractures completely. Irreversibility is explicitly considered with respect to all previous states in the snap-back, leading to a continuous growth of the phase-field during crack-propagation. Alternatively, irreversibility can be considered with respect to the state right before the occurrence of the snap-back, where the peak load is attained. The reader is referred to Alessi et al.⁴² for a detailed comparison between both approaches.

Figure 2(b) shows the evolution of both the elastic energy and the dissipated energy for the single-edge notched specimen subject to tension. In the quasi-linear regime, the dissipated energy is small and almost all energy is elastic. During the snap-back, the elastic energy starts to decrease while the amount of dissipated energy increases. At the end of the loading, all energy is dissipative and the elastic energy vanishes. It can be observed that throughout the loading history, the dissipated energy increases monotonically as a consequence of the dissipation inequality (10), which holds in integral form, and can therefore be used to trace the entire equilibrium path. In case displacements are imposed throughout the entire loading history, the snap-backs would not be captured and, after the phase-field nucleates, the total energy would show a time-discontinuous evolution. As such, the total energy is not conserved and energy balance (9) is not satisfied. This is a consequence of the quasi-static rate-independent evolution, and can be resolved by considering rate-dependent phenomena¹⁴ or by maintaining the rate-independent framework using the present method.

Figure 3 shows the crack phase-field profile for the single-edge notched specimen subject to tension at various time steps. Figure 3(a) shows the nucleation of the crack phase-field at the tip of the notch. Once the crack has nucleated, it propagates to the right (figure 3(b)) without an increase of the vertical displacement (figure 2(a)) and reaches the right edge of the specimen

(figure 3(c)). In case displacements are imposed during the entire loading history, the crack would propagate brutally from the profile in figure 3(a) to the profile in figure 3(c), without an intermediate step.

FIGURE 3 Crack phase-field profile for the single-edge notched specimen subject to tension.

In this example, snap-backs are observed in the equilibrium path of a single-edge notched specimen. Because the specimen is brittle, the dissipation can be expressed in terms of the displacement field and load the multiplier. When the entire equilibrium path is traced, brutal crack propagation is avoided. Alternatively, in case displacements are imposed throughout the entire loading history, a time-discontinuous evolution would occur, which leads to a jump in the total energy and a violation of energy balance. In addition, convergence can no longer be obtained after the peak load is reached. No convergence issues are encountered when a dissipation-based path-following technique is adopted instead. As such, it is observed that by augmenting the governing equations with a dissipation-based path-following constraint, the convergence of the monolithic scheme is enhanced because a time-continuous evolution is recovered and brutal crack propagation is avoided. However, sufficiently small time step sizes are required to achieve convergence with the monolithic scheme.

4.2 | Single-edge notched specimen subject to shear

In this example, the specimen considered in the previous section is loaded horizontally (figure 4) resulting in a crack that propagates less brutally through a region of high tensile stresses. The top edge and side edges are restrained from moving in the vertical direction, while the bottom edge remains completely fixed. In addition, constraint equations are used to constrain the top edge, such that all horizontal displacements are the same. Horizontal displacements are imposed on the top edge in 40 steps of 2×10^{-4} mm, followed by imposing dissipated energy in steps of 10^{-6} J. Similar to the previous example, the displacement and dissipated energy are imposed using the displacement control path-following constraint (19) and dissipation-based path-following constraint (21), respectively. For all time steps, the proposed method results in a response with a positive load multiplier without modifications of the step size t^{prim} . A finite element discretization with 21788 bilinear quadrilateral elements and 21965 nodes is considered, corresponding to an element size $h_c = 0.0027$ mm in the critical zone where fracture is expected to occur. In addition, meshes with different element sizes have been considered, resulting in similar results which are not shown for brevity. In order to prevent volumetric locking in compressed regions of the specimen, a selective reduced integration technique is used to integrate the volumetric term of the elastic energy density in (15c) and the corresponding hydrostatic part of the stress tensor in (15a). A detailed overview and motivation of this procedure can be found in Alessi et al.⁵⁴. For this example, a tolerance $\text{TOL} = 10^{-6}$ is used. On average, the proposed method requires 20.3 iterations per time step, corresponding to a computational time of 29.3 s per time step.

Figure 5(a) shows the equilibrium path for the single-edge notched specimen subject to shear. First, the specimen behaves quasi-linearly, followed by a softening stage and a snap-back. Figure 5(b) shows the evolution of both the elastic energy and the dissipated energy for the single-edge notched specimen subject to shear. Similar to the previous example, the dissipated energy is small in the quasi-linear regime, and starts growing during the softening stage. At the end of the loading history, almost all energy is dissipative. In case displacements would be imposed, a time-discontinuous evolution occurs and the total energy is not conserved.

FIGURE 4 Geometry and boundary conditions of the single-edge notched specimen subject to shear. The dimensions are given in mm.

FIGURE 5 (a) Equilibrium path and (b) energy evolution for the single-edge notched specimen subject to shear. The markers correspond to the time steps at which the crack phase-field is shown in figure 6.

Figure 6 shows the crack phase-field profile for the single-edge notched specimen subject to shear at various time steps. A crack initiates at the tip of the notch, and then propagates through a region of high tensile stresses towards the bottom-right corner. Contrary to the previous example, this example shows a crack that propagates less brutally. However, at the final fracture stage, a snap-back still occurs (figure 5(a)).

FIGURE 6 Crack phase-field profile for the single-edge notched specimen subject to shear.

4.3 | One-dimensional bar subject tension

The example of a one-dimensional bar subject to tension has been studied analytically and numerically using the phase-field approach to ductile fracture by several authors^{42,55,56}. In this example, a bar with a length of 1 mm and a cross-sectional area of 1 mm² is fixed on one side, while a tensile force is applied to the other side. Contrary to the previous two examples, the specimen behaves in a ductile way, governed by an AT-1 model, and has a Young's modulus $E = 1$ MPa, a plastic yield strength $\sigma^p = 1$ MPa, and a local damage dissipation constant $w_0 = 3$ MPa. The response of the bar is computed for several values of the damage length scale $\eta_d \in \{0.0459 \text{ N}^{1/2}, 0.0919 \text{ N}^{1/2}, 0.1837 \text{ N}^{1/2}, 0.3674 \text{ N}^{1/2}\}$ to investigate its influence on the snap-back behavior. These material properties correspond to the ones used by Alessi et al.⁴² (i.e. a damage characteristic length $\ell_d \in \{0.15/8 \text{ mm}, 0.15/4 \text{ mm}, 0.15/2 \text{ mm}, 0.15 \text{ mm}\}$). The Rankine criterion with a tension-compression split in equation (40) is adopted in order to avoid states where the bar is loaded in compression. A uniform finite element discretization with 300 one-dimensional linear elements is considered, corresponding to an element size $h_c = 0.0033$ mm. In addition, meshes with different element sizes have been considered, resulting in similar results which are not shown for brevity. For this example, a tolerance $\text{TOL} = 10^{-9}$ is used. For a damage length scale $\eta_d = 0.0459 \text{ N}^{1/2}$, the proposed method requires, on average, 17.0 iterations per time step, corresponding to a computational time of 66 ms per time step. The performance for the other damage length scales is similar.

Figure 7(a) shows the equilibrium path obtained by elongating the bar in 195 steps of 0.01 mm, followed by controlling the dissipated energy in steps of 10^{-9} J. Contrary to the previous two examples, the dissipated energy can no longer be expressed in terms of the displacement field and the load multiplier only. Therefore, the dissipation-based path-following constraint (20) based on the internal variables is used to control the dissipated energy. The behavior of the bar is initially linear elastic, followed by a perfectly plastic stage, and a coupled damage-plasticity stage. In the coupled damage-plasticity stage, a snap-back occurs, which is more pronounced for smaller damage length scales. This example shows that the dissipation-based path-following constraint (20) allows tracing both the perfectly plastic stage, in which dissipation due to damage is zero, and the coupled damage-plasticity stage, in which dissipation occurs due to both plastic and damage mechanisms. In addition, figure 7(a) shows the equilibrium path of the homogeneous response of the bar, where the plastic strains and the crack phase-field grow uniformly over the length of the bar. This response can be obtained analytically and does not show a snap-back.

FIGURE 7 (a) Equilibrium path computed for different values of $\eta_d \in \{0.0459 \text{ N}^{1/2}, 0.0919 \text{ N}^{1/2}, 0.1837 \text{ N}^{1/2}, 0.3674 \text{ N}^{1/2}\}$, and (b) energy evolution for $\eta_d = 0.0459 \text{ N}^{1/2}$ for the one-dimensional bar subject to tension. In (a), the homogeneous response is shown in blue, the arrow shows the equilibrium paths of a bar with an increasing η_d , and the markers correspond to the time steps at which the plastic strain and crack phase-field are shown in figure 8.

Similar to the first example, the monolithic scheme fails to converge beyond the time step where a snap-back occurs when displacements are imposed throughout the entire loading history using the displacement control path-following constraint (19). However, when the dissipation-based path-following technique is adopted, the entire equilibrium path can be traced without convergence issues.

Figure 7(b) shows the evolution of both the elastic energy and the dissipated energy for the one-dimensional bar subject to tension. Because an AT-1 model is used, the specimen shows an elastic stage. In this stage, the dissipated energy is exactly

zero, and the elastic energy is a quadratic function of the elongation of the bar. In the perfectly plastic stage, the total dissipated energy is a linear function of the elongation, while the elastic energy remains constant. Finally, in the coupled damage-plasticity stage, the dissipated energy increases further and the elastic energy vanishes. If displacements of vanishing time steps would be imposed, the snap-back is not captured and the total energy is not conserved.

Figure 8 shows the profiles of the plastic strain and the crack phase-field at various time steps for a bar with a damage length scale $\eta_d = 0.0459 \text{ N}^{1/2}$. In the perfectly plastic stage, the plastic strains evolve homogeneously, while the crack phase-field remains zero. In the coupled damage-plasticity stage, the crack phase-field and the plastic strains localize in the center of the bar.

FIGURE 8 Profiles of (a) the plastic strain and (b) the crack phase-field for the one-dimensional bar subject to tension with a damage length scale $\eta_d = 0.0459 \text{ N}^{1/2}$.

Contrary to the previous examples, the dissipated energy is expressed in terms of the equivalent plastic strain and the crack phase-field, allowing to capture both the perfectly plastic stage and the coupled damage-plasticity stage. In addition, a Rankine criterion with a tension-compression split is adopted in order to avoid states where the bar is loaded in compression. This example shows that at the end of the perfectly plastic stage, a snap-back occurs, which is more pronounced for smaller damage length scales. When displacements are imposed, a time-discontinuous evolution occurs and the total energy is not conserved.

4.4 | Rectangular specimen subject to tension

The example of a rectangular specimen has been studied using the phase-field approach to ductile fracture by Alessi et al.⁴ and Tanné⁵⁶. In this example, a vertical load is imposed at the top of a rectangular specimen, while the bottom part remains fixed (figure 9). In addition, constraint equations are used to constrain the top edge, such that all vertical displacements are the same. The specimen behaves in a ductile way, governed by an AT-1 model, and has a bulk modulus $K = 0.83 \text{ MPa}$, a shear modulus $G = 0.38 \text{ MPa}$, a plastic yield strength $\sigma^p = 0.5 \text{ MPa}$, a local damage dissipation constant $w_0 = 0.75 \text{ MPa}$, and a damage length scale $\eta_d = 0.13 \text{ N}^{1/2}$, corresponding to a damage characteristic length $\ell_d = 0.106 \text{ mm}$. In addition, plane strain conditions are assumed. A uniform finite element discretization with 13233 bilinear quadrilateral elements and 13450 nodes is considered, corresponding to an element size $h_c = 0.007 \text{ mm}$. Contrary to the previous one-dimensional example, the evolution equations cannot be modified to a Rankine criterion with a tension-compression split and, according to equation (41), the step size t^{prim} will be reduced to prevent states in compression in several time steps. For this example, a tolerance $\text{TOL} = 10^{-7}$ is used. On average, the proposed method requires 24.5 iterations per time step, corresponding to a computational time of 39.4 s per time step.

Figure 10(a) shows the equilibrium path for the rectangular specimen subject to tension obtained by imposing vertical displacements in 90 steps of 0.01 mm, followed by imposing the dissipated energy in steps of 10^{-8} J . Similar to the equilibrium path of the one-dimensional bar (figure 7(a)), the equilibrium path of the rectangular specimen shows an elastic stage, followed by a perfectly plastic stage, and a coupled damage-plasticity stage where a snap-back occurs. Due to the plane strain setting, the

FIGURE 9 Geometry and boundary conditions of the rectangular specimen subject to tension. The dimensions are given in mm.

force is not constant during the perfectly plastic stage. Similar to the previous examples, when the displacement control path-following constraint (19) is used to impose displacements throughout the entire loading history, the monolithic scheme fails to converge beyond the time step where a snap-back occurs. Alternatively, when the dissipation-based path-following technique is adopted, the snap-back is captured and the presented method converges.

Figure 10(b) shows the evolution of both the elastic energy and the dissipated energy for the rectangular specimen subject to tension. Analogous to the example of the one-dimensional bar, the elastic energy is a quadratic function of the displacement of the top edge, and during the perfectly plastic stage, the total dissipated energy is linear. However, in the perfectly plastic stage, the elastic energy is not constant because of the plane strain setting. Finally, in the coupled damage-plasticity stage, the dissipated energy increases further and the elastic energy decreases. When displacements of vanishing time steps are imposed, the snap-back does not occur and the total energy is not conserved.

FIGURE 10 (a) Equilibrium path and (b) energy evolution for the rectangular specimen subject to tension. The markers correspond to the time steps at which the equivalent plastic strain and the crack phase-field are shown in figure 11.

Figure 11 shows the profiles of the equivalent plastic strain and the crack phase-field. Similar to the previous example, the plastic strains are homogeneous in the perfectly plastic stage (figure 11(a)). At this stage, the damage threshold w_0 has not been reached and the damage has not initiated. During the snap-back, a shear band starts to develop in the center of the specimen, and the plastic strains and crack phase-field evolve together (figure 11(b)). In the case where displacements are imposed during the entire loading history, the equivalent plastic strain and the crack phase-field would suddenly change from the profiles in

figure 11(a) to the profiles in figure 11(c), without an intermediate step. When the load is increased, the plastic strains and crack phase-field localize further within the shear band (figure 11(d)).

FIGURE 11 Profiles of the equivalent plastic strain (top) and crack phase-field (bottom) for the rectangular specimen subject to tension.

5 | CONCLUSIONS

In this paper, the system of variational inequalities that governs brittle and ductile fracture processes in phase-field models is augmented with a dissipation-based path-following constraint, and rigorously solved using an interior-point method. By controlling the dissipated energy, the solid is prevented from unloading elastically, and an equilibrium branch with a continuous increase of dissipated energy is followed. As such, the post-peak response of solids loaded by external forces can be captured and snap-backs in the softening stage can be traced. In order to allow for simultaneous dissipation due to both plastic and damage mechanisms, the governing equations are solved monolithically using a novel interior-point method. Because solids can dissipate in both tension and compression, a discontinuous equilibrium path can be obtained when the load multiplier changes sign. Therefore, two novel techniques are presented, which ensure a continuous equilibrium path for which the solid is either in tension or compression.

In case displacements are imposed throughout the entire loading history, time-discontinuous jumps can occur in both the equilibrium path and the total energy, corresponding to brutal crack propagation. Consequently, unaccounted-for rate-dependent phenomena likely occur, and energy balance is violated. However, when snap-backs in the equilibrium path are traced, a non-brutal propagation of cracks can be captured, and energy balance holds throughout. As such, time-discontinuous evolutions are avoided, and it is observed that the convergence of the monolithic scheme is consequently enhanced.

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