# A small deformations effective stress model of gradient plasticity phase-field fracture

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# Abstract

A variational formulation of small strain ductile fracture, based on a phase-field modeling of crack propagation, is proposed. The formulation is based on an effective stress description of gradient plasticity, combined with an AT1 phase-field model. Starting from established variational statements of finite-step elastoplasticity for generalized standard materials, a mixed variational statement is consistently derived, incorporating in a rigorous way a variational finite-step update for both the elastoplastic and the phase-field dissipations. The complex interaction between ductile and brittle dissipation mechanisms is modeled by assuming a plasticity driven crack propagation model. A non-variational function of the equivalent plastic strain is then introduced to modulate the phase-field dissipation based on the developed plastic strains. Particular care has been devoted to the formulation of a consistent Newton-Raphson scheme for the case of Mises plasticity, with a global return mapping and relative tangent matrix, supplemented by a line-search scheme, for the solution of the gradient elastoplasticity problem for fixed phase field. The resulting algorithm has proved to be very robust and computationally effective. Application to several benchmark tests show the robustness and accuracy of the proposed model.

*Keywords:* Phase field, Gradient plasticity, Ductile fracture, Linear complementarity problem, Staggered scheme, Finite element analysis

## 1 1. Introduction

Fracture propagation in elastoplastic solids presents a ductile dissipation mechanism, due to the development of plastic strains, competing and interacting with a brittle dissipation mechanism, due to the generation of new fracture surfaces. The existence of a large scale plastic zone makes Griffith approach to

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<sup>5</sup> brittle fracture inapplicable, as much as its elegant and well-established phase-field variational formulation
<sup>6</sup> introduced in [1, 2]. Several authors have proposed extensions of the phase-field formulation of brittle frac<sup>7</sup> ture incorporating plastic dissipation mechanisms. In the small deformation framework, local plasticity has
<sup>8</sup> been addressed, e.g., in [3, 4, 5, 4, 6, 7, 8, 9], while gradient plasticity mechanisms have been considered
<sup>9</sup> in [10, 11, 12, 13]. In the large deformation framework, the models [14, 15, 16, 17, 18] deal with local
<sup>10</sup> plasticity, while gradient plasticity has been included in the formulation in [19, 20, 21]. A comparative
<sup>11</sup> review of some small-strain ductile fracture models can be found in [22].

In the present work, a variational formulation of small strain ductile fracture, based on a phase-field modeling of crack propagation, is proposed. Starting from established variational statements of finite-step elastoplasticity for generalized standard materials [23, 24, 25, 26, 27, 28, 29], a rather general mixed variational statement, applicable to a wide class of elastoplastic materials, is consistently derived, incorporating in a rigorous way a variational finite-step update for both the elastoplastic and the phase-field dissipations.

The formulation is based on an effective stress [10, 19, 6, 7, 13] description of gradient plasticity, 17 combined with an AT1 phase-field model [30, 31, 17, 16, 13]. The term *effective stress* refers here to the 18 true stress acting on the undamaged portion of the bulk material. The value of the effective stress is then 19 not affected by developing damage. The main consequence of this choice is that plasticity continues to 20 develop until the very final state of material failure, where damage approaches unity. This is in contrast to 21 what happens when plasticity is described in terms of nominal stresses, i.e., when stress are reduced by the 22 current value of damage while the yield stress remains unchanged. In this latter case, as soon as damage 23 starts to develop, the nominal stress decreases and the yield condition is no more satisfied, so that the final 24 part of material deformation is purely brittle (for a discussion on effective vs nominal stresses see, e.g., 25 [6]). It should be noted that other models, where the yield stress is degraded by damage in a way different 26 from the one used for stresses and, therefore, not fitting into the nominal and effective stress classification 27 proposed here, have been presented in the literature (see, e.g., [3, 22, 10]). Unlike for the nominal stress 28 case, for these models it is possible that damage and plasticity evolve together. 29

The fact that effective stresses are used and that plasticity continues to grow also in the damage localization phase, implies that, after damage has started to develop and the global structural response has become softening, incremental plastic strains tend to localize in a one-element-thick band, giving rise to a pathological mesh dependence in the final stage of rupture [21]. To avoid the problem, the simple and effective gradient plasticity regularization proposed in [32] is here adopted. The presence of the gradient plasticity

term introduces computational difficulties for the finite-step time integration of the nonlocal constituive law. 35 A computationally effective and robust Newton-Raphson scheme for the solution of the gradient elastoplas-36 tic problem for fixed damage is therefore proposed for the case of Mises plasticity, together with its global 37 return mapping algorithm and expression of the global consistent tangent matrix. This global return map-38 ping scheme allows to formulate the finite-step elastoplastic problem as a global linear complementarity 39 problem. The same has been done for the phase-field problem, so that irreversibility of both plastic and 40 brittle dissipation turns out to be enforced in a rigorous way. Both linear complementarity problems have 41 been solved using a very efficient explicit Projected Successive Over-Relaxation (PSOR) algorithm [33], 42 following the approach proposed in [32, 34]. 43

In ductile fracture, either already existing voids, or voids nucleated under the effect of developing plastic 44 strains at inclusions or second-phase particles, grow until they coalesce giving rise to a continuous fracture 45 path. Voids nucleation and growth is associated to locally high levels of plastic deformation, suggesting 46 that in most cases ductile fracture requires high levels of energy absorption (see, e.g., [35]). Based on these 47 physical observations, in the proposed phase-field plasticity model, crack nucleation and propagation is 48 assumed to be driven by plasticity. Damage development is then possible when the plastic process zone in 49 a stress concentration region reaches a critical level, measured by the equivalent plastic strain. In practical 50 terms, this is achieved in the model by introducing in the damage activation condition a non-variational 51 function of the equivalent plastic strain, modulating the effective value of the material fracture energy. This 52 is somehow in line with what has been done by several other authors ([7, 9, 17]), though making use of 53 substantially different definition of the fracture energy modulation function. Another important aspect, а 54 clearly emerging from the considered numerical applications, is the capability of the proposed plasticity 55 driven approach to predict crack nucleation in the absence of a pre-existing crack (for a discussion on 56 phase-field prediction of crack nucleation see, e.g., [36, 37]). 57

The AT1 model used here has some key conceptual and practical advantages over the AT2 model: it has a non-zero elastic limit, preventing diffuse damage at small loading and the damage localization band is of finite width [36]. Both features are of importance in the considered plasticity driven framework: i) the material response remains linear elastic until the yield limit is achieved, without any damage development; ii) having a finite width, it is possible to define the phase-field characteristic length so that the phase-field localization band remains entirely contained within the plasticity process zone.

<sup>64</sup> The paper is organized as follows. In Section 2 the phase-field model to ductile fracture is built starting

from a consistent thermodynamic formulation in rate form. Then, the discrete finite-step governing equa-65 tions and evolution laws are derived with a Hu-Washizu variational approach. Finally, the main constitutive 66 choices are presented. In Section 3 the fracture activation criterion is modified with the introduction of a 67 non-variational modulation function f. Its optimal profile is derived based on a 1D homogeneus model and 68 the meaning of the additional material parameters is discussed. In Section 4 the spatial discretization of 69 the governing equations is performed. In Section 5 algorithmic aspects, such as the alternate minimization 70 scheme and the elastoplastic monolithic scheme, are detailed. In Section 6 numerical applications to several 71 benchmark problems are presented and discussed. 72

## 73 2. Phase-field ductile fracture

#### 74 2.1. Nominal & effective responses

Let  $\Omega_0 \subset \mathbb{R}^{n_{dim}}$  be the reference domain, where  $n_{dim}$  is the problem dimension. It is subject to Dirichelet 75 boundary conditions on  $\partial \Omega_D$  and Neumann boundary conditions on  $\partial \Omega_N$  with  $\partial \Omega_D \cup \partial \Omega_N = \partial \Omega_0$  and 76  $\partial \Omega_D \cap \partial \Omega_N = \emptyset$ . The displacement field **u** is subject to **u** = **u**<sub>D</sub> on  $\partial \Omega_D$ . The phase-field damage-77 like variable d is a scalar quantity ranging from 0 to 1 interpolating the unbroken and fully broken state 78 of the material, respectively. The material degradation function  $\omega(d)$ , also often referred to as *continuity* 79 *function*, accounts for the presence of damage in the material bulk and it is such that  $\omega(0) = 1$ ,  $\omega(1) = 0$ 80 and  $\omega'(d) < 0$ . In the damaged state,  $d\Omega_0$  defines the infinitesimal nominal volume, equal to the original 81 undamaged volume, while  $d\Omega = \omega \ d\Omega_0$  is the current effective volume, i.e., the nominal volume minus 82 the volume of the defects. A sketch of the different volumes is shown in Figure 1, where  $\Omega_V$  is the micro-83 voids volume. Note that, while  $\Omega_0$  denotes the nominal volume and  $\Omega$  the effective one, in what follows 84 the effective quantities, i.e., quantities referred to the damaged volume, are always denoted with a zero 85 subscript  $(\cdot)_0$ , while the nominal quantities, i.e., those referred to the undamaged volume, do not have a zero 86 subscript. The pointwise transformation from effective to nominal quantity reads: 87

$$\underbrace{(\cdot)_{0}}_{effective} \underbrace{d\Omega}_{effective} = \underbrace{(\cdot)_{0}}_{effective} \omega \underbrace{d\Omega_{0}}_{nominal} = \underbrace{(\cdot)}_{nominal} \underbrace{d\Omega_{0}}_{nominal}$$
(1)



Figure 1: Nominal  $\Omega_0$ , voids  $\Omega_V$ , and effective  $\Omega$  volumes

## 88 2.2. State variables & evolution laws

An elastoplastic material, belonging to the class of generalized standard materials [38], is considered. 89 The material state is assumed to be completely defined by the total strain tensor  $\varepsilon := \nabla^s \mathbf{u} (\nabla^s(\cdot))$  being 90 the symmetric gradient operator), the plastic strain tensor  $\varepsilon^p$ , the hardening internal variable  $\alpha$ , and the 91 damage-like phase field d. The free energy  $\psi$  density is assumed to be additively decomposed into its elas-92 tic (reversible) part  $\omega \psi_0^e(\varepsilon^e)$ ,  $\varepsilon^e = \varepsilon - \varepsilon^p$  denoting the elastic strain tensor, and hardening (unrecoverable) 93  $\omega \psi_0^p(\alpha)$  part, the latter being the internal elastic energy stored in the material because of irreversible de-94 formations of the microstructure. The energies  $\psi_0^e(\varepsilon^e)$  and  $\psi_0^p(\alpha)$ , assumed to be convex functions of their 95 arguments, are the undamaged or effective elastic and hardening free energies. The nominal and effective 96 free energy densities are defined as: 97

$$\psi := \omega \psi_0 \quad , \quad \psi_0 := \psi_0^e + \psi_0^p$$
 (2)

The Clausius-Duhem inequality states that the specific dissipation rate  $\dot{\phi}$  must increase in every transformation, i.e.  $\dot{\phi} := \sigma : \dot{\varepsilon} - \dot{\psi} \ge 0$ , where  $\sigma$  is the Cauchy stress tensor,  $\dot{\varepsilon}$  is the total strain rate, and  $\dot{\psi}$  is the free energy rate. The introduction of (2) into the dissipation inequality reads:

$$\dot{\phi} := \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\psi} = \underbrace{(\boldsymbol{\sigma} - \omega \,\partial_{\boldsymbol{\varepsilon}^e} \psi_0^e) : \dot{\boldsymbol{\varepsilon}}^e}_{elastic} + \underbrace{\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \omega \,\partial_{\boldsymbol{\alpha}} \psi_0^p \,\dot{\boldsymbol{\alpha}}}_{plastic} - \underbrace{\boldsymbol{\omega}' \,\psi_0 \,\dot{\boldsymbol{d}}}_{fracture} \ge 0 \tag{3}$$

During an elastic or reversible transformation, no evolution of the plastic deformations  $\dot{\boldsymbol{\varepsilon}}^p = \mathbf{0}$ , of the hardening variable  $\dot{\alpha} = 0$  or of damage  $\dot{d} = 0$  occurs and, hence, no dissipation increase is produced (i.e.,  $\dot{\phi} = 0$ ). Therefore, the only term left is  $(\boldsymbol{\sigma} - \omega \partial_{\boldsymbol{\varepsilon}} \psi_0^e)$  :  $\dot{\boldsymbol{\varepsilon}} = 0$ . Since it must hold for all reversible transformations  $\dot{\boldsymbol{\varepsilon}}$ , the nominal and effective elastic evolution laws read:

$$\boldsymbol{\sigma} = \omega \, \boldsymbol{\sigma}_0 \quad , \quad \boldsymbol{\sigma}_0 := \partial_{\boldsymbol{\varepsilon}^e} \boldsymbol{\psi}_0^e \tag{4}$$

<sup>105</sup> Consideration of the dissipation inequality in the conditions of no damage,  $\dot{d} = 0$ , allows to define:

$$\dot{\phi}^p = \omega \, \dot{\phi}^p_0 \quad , \quad \dot{\phi}^p_0 := \boldsymbol{\sigma}_0 : \dot{\boldsymbol{\varepsilon}}^p - \chi_0 \cdot \dot{\alpha} \ge 0 \tag{5}$$

where  $\dot{\phi}_0^p$  denotes the dissipation rate due to plasticity only and  $\chi_0$  is the effective *static* hardening variable, i.e. the thermodynamic force work-conjugated to the internal variable  $\alpha$ . From (3), it turns out to be defined as:

$$\chi_0 := \partial_\alpha \psi_0^p \tag{6}$$

The elastoplastic dissipation inequality  $(5)_2$  can be also expressed in terms of its effective counterpart, i.e., 109  $\dot{\phi}^p d\Omega_0 = \dot{\phi}_0^p d\Omega \ge 0$ . The effective yield stress associated to the internal variable  $\alpha$  is  $\sigma_{y0}(\alpha) = \bar{\sigma}_{y0} + \chi_0(\alpha)$ , 110 where  $\bar{\sigma}_{y0}$  is the initial yield stress. The elastoplastic evolution has to satisfy the additional constraint 111 that the admissible set of effective stress and hardening parameter ( $\sigma_0^*, \chi_0^*$ ) has to fullfil the yield criterion 112  $f_y(\sigma_0^*, \chi_0^*) \le 0$ , where  $f_y$  is the local yield function, convex in the space of stress and static internal variable. 113 The yield criterion is postulated in terms of effective quantities, since only the continuous, non-damaged part 114 of the volume is undergoing plastic deformations. The stationarity conditions associated to the (effective) 115 principle of maximum dissipation provide the effective elastoplastic evolution laws: 116

$$\dot{\boldsymbol{\varepsilon}}^{p} = \dot{\lambda} \partial_{\boldsymbol{\sigma}_{0}} f_{y} \quad , \quad \dot{\boldsymbol{\alpha}} = -\dot{\lambda} \partial_{\chi_{0}} f_{y} \quad , \quad \dot{\lambda} \ge 0 \quad , \quad f_{y} \le 0 \quad , \quad \dot{\lambda} f_{y} = 0 \tag{7}$$

where  $\dot{\lambda}$  is the non-negative rate of a scalar plastic multiplier. Finally, the ductile-fracture specific dissipation rate  $\dot{\phi}^{pf}$  reads:

$$\dot{\phi}^{pf} := \omega \,\dot{\phi}^p_0 + \dot{\phi}^f \quad , \quad \dot{\phi}^f := G \,\dot{d} \quad , \quad G := -\omega' \,\psi_0 \tag{8}$$

where the  $\dot{\phi}^{f}$  is the brittle fracture specific dissipation rate and *G* is the fracture driving force.  $\dot{\phi}^{pf}$  is the dissipation rate per unit nominal volume and, therefore, the elementary dissipation rate is  $\dot{\phi}^{pf} d\Omega_{0}$ .

# 121 2.3. Variational formulation of the finite-step problem

## 122 2.3.1. Elastoplastic variational update

Let us first consider an elastoplastic material without damage. In this case, effective and nominal quantities coincide, since there are no developing defects inside the volume. The subscript 0 will be therefore used only for homogeneity with the subsequent sections. Let  $\Delta w_0^{int}$  be the specific elastoplastic internal work carried out along a deformation process between time  $t^n$  and  $t^{n+1}$ 

$$\Delta w_0^{int} = \int_{t^n}^{t^{n+1}} \boldsymbol{\sigma}_0 : \dot{\boldsymbol{\varepsilon}} dt = \int_{t^n}^{t^{n+1}} \left[ \boldsymbol{\sigma}_0 : \dot{\boldsymbol{\varepsilon}}^e + \chi_0 \dot{\alpha} + (\boldsymbol{\sigma}_0 : \dot{\boldsymbol{\varepsilon}}^p - \chi_0 \dot{\alpha}) \right] dt = \Delta \psi_0^e + \Delta \psi_0^p + \Delta \phi_0^p \tag{9}$$

where the symbol  $\Delta(\cdot)$  denotes the increment of the quantity (·) over the time step  $\Delta t = t^{n+1} - t^n$ . We define an extremal path as a path in strain space from  $\varepsilon^n = \varepsilon(t^n)$  to  $\varepsilon^{n+1} = \varepsilon(t^{n+1})$ ,  $\varepsilon^n$  and  $\varepsilon^{n+1}$  being prescribed strains, minimizing the internal work  $\Delta w_0^{int}$ . Let  $\Delta \bar{w}_0^{int}$  be the minimum value of  $\Delta w_0^{int}$ , so that  $\Delta w_0^{int} \ge \Delta \bar{w}_0^{int}$ along any strain path from  $\boldsymbol{\varepsilon}^n$  to  $\boldsymbol{\varepsilon}^{n+1}$ .

Since  $\Delta \psi_0^e$  and  $\Delta \psi_0^p$  are path independent quantities, they take the same value along any path between  $\epsilon^n$  and  $\epsilon^{n+1}$  and the extremal path minimizes  $\Delta \phi_0^p$ . Let  $\Delta \bar{\phi}_0^p$  be this minimum value. Obviously, if a feasible purely elastic path exists from  $\epsilon^n$  to  $\epsilon^{n+1}$ , this is an extremal path. While the sum  $\Delta \epsilon = \epsilon^{n+1} - \epsilon^n = \Delta \epsilon^e + \Delta \epsilon^p$ is prescribed, different paths lead to different increments of elastic and plastic strains. The extremal path is therefore the solution of the following minimization problem:

$$\Delta \bar{w}_0^{int} = \min_{\Delta \varepsilon^e, \Delta \varepsilon^p, \Delta \alpha} \{ \Delta \psi_0^e + \Delta \psi_0^p + \Delta \phi_0^p \mid \Delta \varepsilon^e + \Delta \varepsilon^p = \Delta \varepsilon \}$$
(10)

where the total strain increment  $\Delta \varepsilon$  is prescribed.

Based on the principle of maximum dissipation, it has been shown [23, 24] that, for prescribed incre-137 ments of  $\Delta \varepsilon^p$  and  $\Delta \alpha$  over the time step, extremal paths in the plastic variables space (i.e., leading to the 138 minimum increment of dissipation  $\Delta \bar{\phi}_0^p$ ) are obtained by letting  $\varepsilon^p$  and  $\alpha$  evolve only at constant stress, as it 139 is the case when a backward-difference time integration of the elastoplastic constitutive law (often referred 140 to as return mapping algorithm) is adopted. In this case, the step can be seen to have been elastic until 141 the end of the step and plastic evolution is allowed only when the final values  $\sigma_0^{n+1}$  and  $\chi_0^{n+1}$  have been 142 achieved (see [28] for a review of extremum properties of the generalized midpoint time integration rule). 143 The backward-difference integrated conditions defining the extremal path, i.e. its optimality conditions, are 144 given by (with  $f_y^{n+1} = f_y(\sigma_0^{n+1}, \chi_0^{n+1})$ ): 145

$$\Delta \boldsymbol{\varepsilon}^{p} = \Delta \lambda \,\partial_{\boldsymbol{\sigma}_{0}} f_{y}^{n+1} \quad , \quad \Delta \alpha = -\Delta \lambda \,\partial_{\chi_{0}} f_{y}^{n+1} \quad , \quad \Delta \lambda \ge 0 \quad , \quad f_{y}^{n+1} \le 0 \quad , \quad \Delta \lambda \cdot f_{y}^{n+1} = 0 \tag{11}$$

while the backward-difference finite-step version of the principle of maximum dissipation reads

$$\Delta \bar{\phi}_0^p = \max_{\boldsymbol{\sigma}_0^{n+1}, \chi_0^{n+1} \in f_y \le 0} \{ \boldsymbol{\sigma}_0^{n+1} : \Delta \boldsymbol{\varepsilon}^p - \chi_0^{n+1} \Delta \alpha \}$$
(12)

For the considered class of generalized standard materials, the backward-difference integration algorithm has also been shown to preserve the symmetry of the consistent tangent, implying the existence of an incremental potential  $\bar{w}_0^{int\,n}$  such that  $\sigma_0^{n+1} = \partial \bar{w}_0^{int\,n} / \partial \varepsilon^{n+1}$  [24]. In view of the special extremal property of the backward-difference integrated elastoplastic constitutive law, this time-integration scheme will be adopted throughout this work and the symbol  $\Delta \phi_0^p$  (without the bar) will be used to denote its corresponding plastic dissipation increment over the time step. Assuming that the solution of the elastoplastic problem is known at time  $t^n$ , this choice of the integration scheme allows for a variational characterization of the solution of the finite-step elastoplastic problem, which can be shown to coincide with the solution of the
 following constrained minimization problem [26, 27, 28]:

$$\min_{\mathbf{u},\Delta\varepsilon} \left\{ \Pi_p^n = \int_{\Omega_0} \left( \psi_0^{n+1} + \Delta \phi_0^p \right) d\Omega_0 - \mathcal{W}^{n+1} \right\}$$
(13)

156 where

$$\psi_0^{n+1} = \psi_0^e \left( \boldsymbol{\varepsilon}^{e\,n} + \Delta \boldsymbol{\varepsilon}^e \right) + \psi_0^p \left( \boldsymbol{\alpha}^n + \Delta \boldsymbol{\alpha} \right) \tag{14}$$

157 W denotes the external work and the functional is subjected to the compatibility conditions

$$\boldsymbol{\varepsilon}^{n} + \Delta \boldsymbol{\varepsilon}^{e} + \Delta \boldsymbol{\varepsilon}^{p} = \boldsymbol{\varepsilon}^{n+1} = \boldsymbol{\nabla}^{s} \mathbf{u}^{n+1}, \quad \mathbf{u}^{n+1} = \bar{\mathbf{u}}^{n+1} \text{ on } \partial \Omega_{D}$$
(15)

 $\bar{\mathbf{u}}^{n+1}$  being prescribed displacement values at  $t = t^{n+1}$  on the constrained boundary  $\partial \Omega_D$ . In (13),  $\Delta \phi_0^p$  is the extremal dissipation increment resulting from application of the return mapping algorithm.

The minimum problem in (13) can be expressed in a more explicit form by writing its associated Lagrangian functional [25, 29]:

$$\mathcal{L}_{p}^{n}(\mathbf{u}^{n+1},\Delta\boldsymbol{\varepsilon}^{e},\Delta\boldsymbol{\varepsilon}^{p},\Delta\boldsymbol{\alpha},\boldsymbol{\sigma}_{0}^{n+1},\Delta\boldsymbol{\lambda}) = \Pi_{p}^{n} - \int_{\Omega_{0}} f_{y}\left(\Delta\boldsymbol{\varepsilon}^{e},\Delta\boldsymbol{\alpha}\right)\Delta\boldsymbol{\lambda}\,d\Omega_{0} - \int_{\Omega_{0}} \boldsymbol{\sigma}_{0}^{n+1} : \left[\boldsymbol{\varepsilon}^{e\,n} + \boldsymbol{\varepsilon}^{p\,n} + \Delta\boldsymbol{\varepsilon}^{e} + \Delta\boldsymbol{\varepsilon}^{p} - \boldsymbol{\nabla}^{s}\mathbf{u}^{n+1}\right]d\Omega_{0},$$
(16)

subject to  $\Delta \lambda \ge 0$  and  $\mathbf{u}^{n+1} = \bar{\mathbf{u}}^{n+1}$  on  $\partial \Omega_D$ .

In (16),  $\sigma_0^{n+1}$  (not sign-constrained) and  $\Delta \lambda \ge 0$  play the role of Lagrange multipliers for the compatibility and plastic admissibility constraints. It is easy to verify that the solution of the finite-step elastoplastic boundary value problem is given by the solution of the following variational problem, where the last condition is a variational inequality due to the sign constraint on  $\Delta \lambda$ :

$$\begin{aligned} \partial_{\mathbf{u}} \mathcal{L}_{p}^{n}[\delta \mathbf{u}] &= 0 \qquad \forall \, \delta \mathbf{u}, \text{ with } \delta \mathbf{u} = 0 \text{ on } \partial \Omega_{D} \\ \partial_{\Delta \varepsilon^{e}} \mathcal{L}_{p}^{n}[\delta \Delta \varepsilon^{e}] &= 0 \qquad \forall \, \delta \Delta \varepsilon^{e} \\ \partial_{\Delta \varepsilon^{p}} \mathcal{L}_{p}^{n}[\delta \Delta \varepsilon^{p}] &= 0 \qquad \forall \, \delta \Delta \varepsilon^{p} \\ \partial_{\Delta \alpha} \mathcal{L}_{p}^{n}[\delta \Delta \alpha] &= 0 \qquad \forall \, \delta \Delta \alpha \\ \partial_{\sigma_{0}} \mathcal{L}_{p}^{n}[\delta \sigma_{0}^{n+1}] &= 0 \qquad \forall \, \delta \sigma_{0}^{n+1} \\ \partial_{\Delta \lambda} \mathcal{L}_{p}^{n}[\delta \lambda] \geq 0 \qquad \forall \, \delta \lambda = \Delta \lambda' - \Delta \lambda, \text{ with } \Delta \lambda' \geq 0 \text{ and } \Delta \lambda \geq 0 \end{aligned}$$

$$(17)$$

#### 167 2.3.2. Phase-field finite-step variational formulation of ductile fracture

To account for the propagation of fracture driven by the development of localized plasticity, the func-168 tional  $\mathcal{L}_p^n$  in (16) is enriched by the addition of the energy dissipated by the damage-like phase field d, 169 responsible for the material stiffness and strength degradation. Since in the presence of softening struc-170 tural response plastic strains tend to localize in a zero-thickness band, a further regularization of the model 17 becomes necessary (see, e.g., [10, 19, 12, 13, 20]). A common and effective provision, motivated by mi-172 croscale considerations (see, e.g., [39, 40]) consists in introducing into the model a diffusive term of an 173 inelastic, irreversible quantity (see, e.g., [41, 42]). The simple and effective gradient formulation of finite-174 step elastoplasticity presented in [32] is considered here. Defining the set 175

$$S := (\mathbf{u}, \boldsymbol{\varepsilon}, \Delta \boldsymbol{\varepsilon}^{p}, \boldsymbol{\sigma}_{0}, \boldsymbol{\sigma}_{0}^{p}, \chi_{0}, \Delta \boldsymbol{\alpha}, \Delta \boldsymbol{\lambda}, \Delta \boldsymbol{d})$$
(18)

of independent fields, the new, gradient-enriched functional  $\mathcal{L}_{pd}^{\nabla n}(S)$  is defined below. The stress field  $\sigma_0^p$ in S is a dummy field considered to facilitate the derivation of the governing equations resulting from the stationarity of the functional. For all quantities evaluated at time  $t^{n+1}$ , the n+1 at exponent has been omitted for notation convenience:

$$\mathcal{L}_{pd}^{\nabla n} := \int_{\Omega_{0}} \omega(d) \left[ \psi_{0}^{e} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{p\,n} - \Delta \boldsymbol{\varepsilon}^{p}) + \psi_{0}^{p} (\alpha^{n} + \Delta \alpha) \right] d\Omega_{0} - \int_{\Omega_{0}} \mathbf{b} \cdot \mathbf{u} \, d\Omega_{0} - \int_{\partial\Omega_{N}} \mathbf{t} \cdot \mathbf{u} \, d\Gamma + \int_{\text{stored internal energy } \mathcal{E}} \psi_{0}^{p} (\alpha^{n} + \Delta \alpha) d\Omega_{0} - \int_{\Omega_{0}} \mathbf{b} \cdot \mathbf{u} \, d\Omega_{0} - \int_{\partial\Omega_{N}} \mathbf{t} \cdot \mathbf{u} \, d\Gamma + \int_{\Omega_{0}} \omega(d) \left( \boldsymbol{\sigma}_{0}^{p} : \Delta \boldsymbol{\varepsilon}^{p} - \chi_{0} \, \Delta \alpha \right) d\Omega_{0} + \int_{\Omega_{0}} \phi^{f} (d, \nabla d) \, d\Omega_{0} + \int_{\Omega_{0}} \frac{\eta_{f}}{2 \, \Delta t} \left( \Delta d \right)^{2} \, d\Omega_{0} + \int_{\text{plastic dissipation increment } \Delta \mathcal{D}^{p}} \int_{\text{fracture energy } \mathcal{D}_{f}} \psi_{\text{iscous energy } \mathcal{D}_{V}} (\Delta d)^{2} \, d\Omega_{0} + \int_{\Omega_{0}} \omega(d) \, \boldsymbol{\sigma}_{0} : (\nabla^{s} \mathbf{u} - \boldsymbol{\varepsilon}) \, d\Omega_{0} - \int_{\Omega_{0}} \omega(d) \, \Delta \lambda \, f_{y}(\boldsymbol{\sigma}_{0}^{p}, \chi_{0}) \, d\Omega_{0} + \int_{\Omega_{0}} \omega(d) \, \frac{1}{2} \, c_{p} \, \nabla \lambda \cdot \nabla \lambda \, d\Omega_{0} + \int_{\text{compatibility constraint}} \psi_{\text{plastic admissibility}} (\Delta d)^{2} \, d\Omega_{0} + \int_{\Omega_{0}} \omega(d) \, \frac{1}{2} \, c_{p} \, \nabla \lambda \cdot \nabla \lambda \, d\Omega_{0} + \int_{\Omega_{0}} \psi_{plastic admissibility} (\Delta d)^{2} \, d\Omega_{0} + \int_{\Omega_{0}} \psi_{plastic admissibility} (\Delta d)$$

180 subject to

$$\Delta \lambda \ge 0, \quad \Delta d \ge 0, \quad \mathbf{u} = \bar{\mathbf{u}} \text{ on } \partial \Omega_D$$

$$\tag{20}$$

The notion of effective volume enters in the definition of the volume integrals. With the exception of the fracture energy  $\mathcal{D}_f$  and of the external work  $\mathcal{W}$ , the energies and the constraints are defined on the continuous portion of the material volume  $\Omega$  only, hence  $\int_{\Omega} (\cdot)_0 d\Omega = \int_{\Omega_0} \omega (\cdot)_0 d\Omega_0$ ,  $\Omega_0$  being the reference nominal volume. The vectors **b** and **t** are the body forces and the tractions, respectively, applied on the Neumann portion  $\partial \Omega_N$  of the boundary. In the standard phase-field formulation,

$$\phi^{f}(d, \nabla d) = w(d) + \frac{1}{2}c_{d} \nabla d \cdot \nabla d$$
(21)

where w(d) is the local phase-field specific dissipation. The constant parameters  $c_p$  and  $c_d$  measure the plastic and damage diffusion bandwidths and they are related to the plastic and fracture internal lengths  $l_{0p}$ and  $l_{0d}$ . The viscous coefficient  $\eta_f$  introduces a pseudo-time measure of the crack propagation rate, while  $\Delta t = t^{n+1} - t^n$  is the current time-step size. This dissipative term is introduced for algorithmic reasons, as it will be discussed later. The solution of the considered ductile fracture boundary value problem makes the functional  $\mathcal{L}_{pd}^{\nabla n}(S)$  stationary with respect to variations of the fields in S. The inequality constraints on  $\Delta\lambda$ and  $\Delta d$  make the variational problem a variational inequality.

#### 193 2.3.3. Stationarity conditions

<sup>194</sup> The stationarity conditions for  $\mathcal{L}_{pd}^{\nabla n}(\mathcal{S})$  read:

$$\partial_{\mathbf{u}} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta \mathbf{u}] = 0 \quad \rightarrow \quad \int_{\Omega_0} \omega \, \boldsymbol{\sigma}_0 : \boldsymbol{\nabla}^s \delta \mathbf{u} \, \mathrm{d}\Omega_0 - \int_{\Omega_0} \mathbf{b} \cdot \delta \mathbf{u} \, \mathrm{d}\Omega_0 - \int_{\partial \Omega_N} \mathbf{t} \cdot \delta \mathbf{u} \, \mathrm{d}\Gamma = 0 \tag{22a}$$

$$\partial_{\varepsilon} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta \varepsilon] = 0 \quad \to \quad \int_{\Omega_0} \omega \left( \partial_{\varepsilon} \psi_0^e - \sigma_0 \right) : \delta \varepsilon \, \mathrm{d}\Omega_0 = 0 \tag{22b}$$

$$\partial_{\sigma_0} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta \sigma_0] = 0 \quad \to \quad \int_{\Omega_0} \omega \left( \nabla^s \mathbf{u} - \boldsymbol{\varepsilon} \right) : \delta \sigma_0 \, \mathrm{d}\Omega_0 = 0 \tag{22c}$$

$$\partial_{\alpha} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta\alpha] = 0 \quad \to \quad \int_{\Omega_0} \omega \left( \partial_{\alpha} \psi_0^p - \chi_0 \right) \delta\alpha \, \mathrm{d}\Omega_0 = 0 \tag{22d}$$

$$\partial_{\varepsilon^{p}} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta \varepsilon^{p}] = 0 \quad \to \quad \int_{\Omega_{0}} \omega \left( -\partial_{\varepsilon} \psi_{0}^{e} + \sigma_{0}^{p} \right) : \delta \varepsilon^{p} \, \mathrm{d}\Omega_{0} = 0 \tag{22e}$$

$$\partial_{\sigma_0^p} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta \sigma_0^p] = 0 \quad \to \quad \int_{\Omega_0} \omega \left( \Delta \varepsilon^p - \Delta \lambda \ \partial_{\sigma_0^p} f_y \right) : \delta \sigma_0^p \, \mathrm{d}\Omega_0 = 0 \tag{22f}$$

$$\partial_{\chi_0} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta\chi_0] = 0 \quad \to \quad \int_{\Omega_0} -\omega \left( \Delta \alpha + \Delta \lambda \ \partial_{\chi_0} f_y \right) \delta\chi_0 \, \mathrm{d}\Omega_0 = 0 \tag{22g}$$

$$\partial_{\lambda} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta\lambda] \ge 0 \quad \to \quad \int_{\Omega_0} \omega \left[ -\delta\lambda f_y + c_p \, \nabla \lambda \cdot \nabla \delta\lambda \right] \mathrm{d}\Omega_0 \ge 0 \tag{22h}$$

$$\partial_{d} \mathcal{L}_{pd}^{\nabla n}(\mathcal{S})[\delta d] \ge 0 \quad \to \quad \int_{\Omega_{0}} \left\{ \left[ \omega' \,\tilde{\psi}_{0} + w' + \frac{\eta_{f}}{\tau} \,\Delta d \right] \delta d + c_{d} \,\nabla d \cdot \nabla \delta d \right\} \,\mathrm{d}\Omega_{0} \ge 0, \tag{22i}$$

where  $\delta \lambda = \Delta \lambda' - \Delta \lambda$ ,  $\delta d = \Delta d' - \Delta d$  are not sign-constrained, while  $\Delta \lambda' \ge 0$ ,  $\Delta d' \ge 0$  are aribitrary, non-negative scalar functions belonging to the same spaces of  $\Delta \lambda$  and  $\Delta d$ , respectively, and

 $\Delta \lambda \ge 0, \quad \Delta d \ge 0, \quad \mathbf{u} = \bar{\mathbf{u}} \text{ on } \partial \Omega_D$ 

<sup>197</sup> The driving energy  $\tilde{\psi}_0$  in (22i) is defined as

$$\tilde{\psi}_0(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}_0^p, \chi_0, \alpha, \lambda) := \psi_0(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \alpha) + \Delta \phi_0^p(\boldsymbol{\varepsilon}^p, \boldsymbol{\sigma}_0^p, \chi_0, \alpha) - f_y(\boldsymbol{\sigma}_0^p, \chi_0) \,\Delta \lambda + \frac{1}{2} \, c_p \, \boldsymbol{\nabla} \lambda \cdot \boldsymbol{\nabla} \lambda \tag{23}$$

It contains the term  $f_y \Delta \lambda$  that is non-vanishing due to the gradient plasticity term. The conditions above correspond to: (22a) equilibrium equations, (22b) elastic state equations, (22c) compatibility conditions, (22d) static hardening variable state equation, (22e) (together with (22b)) identity between the dummy stress  $\sigma_0^p$  and the effective stress  $\sigma_0$ , (22f) plastic strains evolution, (22g) hardening variable evolution, (22h) non-local plastic consistency, (22i) non-local fracture evolution criterion. To simplify the notation in what follows, the symbols  $\alpha$ ,  $\lambda$ , d are used to express the functional dependencies, rather than the corresponding increments  $\Delta \alpha$ ,  $\Delta \lambda$ ,  $\Delta d$  as already done in (23).

#### 205 2.3.4. Governing equations of the non-local problem

In the implemented formulation, the compatibility condition (22c) is enforced in strong form, i.e.  $\varepsilon = \nabla_s \mathbf{u}$  as in standard compatible finite elements, and the dummy stress field  $\sigma_0^p$  is eliminated assuming  $\sigma_0^p \equiv \sigma_0$ . Equation (22a), combined with the compatibility condition (22c), leads to the weak form of the momentum balance equation, expressed in terms of nominal quantities:

$$\int_{\Omega_0} \omega \,\boldsymbol{\sigma}_0 : \delta \boldsymbol{\varepsilon} \, \mathrm{d}\Omega_0 = \int_{\Omega_0} \mathbf{b} \cdot \delta \mathbf{u} \, \mathrm{d}\Omega_0 + \int_{\partial \Omega_N} \mathbf{t} \cdot \delta \mathbf{u} \, \mathrm{d}\Gamma$$
(24)

The stationarity conditions (22b), (22d)-(22g), lead to the effective local state equations and elastoplastic evolution laws:

$$\boldsymbol{\sigma}_0 = \partial_{\boldsymbol{\varepsilon}} \boldsymbol{\psi}_0^e \quad , \quad \boldsymbol{\chi}_0 = \partial_{\alpha} \boldsymbol{\psi}_0^p \quad , \quad \Delta \boldsymbol{\varepsilon}^p = \Delta \lambda \, \partial_{\boldsymbol{\sigma}_0} f_y \quad , \quad \Delta \alpha = -\Delta \lambda \, \partial_{\boldsymbol{\chi}_0} f_y \tag{25}$$

while the corresponding nominal stress and static internal variable are obtained as  $\sigma = \omega \sigma_0$ ,  $\chi = \omega \chi_0$ .

While the variations (22a)-(22g) are standard equalities, (22h) and (22i) are variational inequalities. Using standard arguments for variational inequalities, condition (22h) can be written in the following equivalent form defining the elastoplastic non-local loading-unloading conditions:

$$\Delta \lambda \ge 0 \quad , \quad \mathcal{F}_{y}(\boldsymbol{\sigma}_{0}, \chi_{0}, \lambda, d) \le 0 \quad , \quad \mathcal{F}_{y}(\boldsymbol{\sigma}_{0}, \chi_{0}, \lambda, d)[\Delta \lambda] = 0$$
(26)

where the non-local yield functional  $\mathcal{F}_y$  has been defined as:

$$\mathcal{F}_{y}(\boldsymbol{\sigma}_{0},\chi_{0},\lambda,d)[\delta\lambda] := \int_{\Omega_{0}} \omega(d) \left[ f_{y}(\boldsymbol{\sigma}_{0},\chi_{0}) \,\delta\lambda - c_{p} \,\boldsymbol{\nabla}\lambda \cdot \boldsymbol{\nabla}\delta\lambda \right] \mathrm{d}\Omega_{0}$$
(27)

Similarly, the energy release rate G and critical energy release rate  $G_c$  functionals are defined as:

$$\mathcal{G}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{p}, \boldsymbol{\alpha}, \boldsymbol{\lambda}, d)[\delta d] := -\int_{\Omega_{0}} \omega'(d) \,\tilde{\psi}_{0}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{p}, \boldsymbol{\alpha}, \boldsymbol{\lambda}) \,\delta d \,\mathrm{d}\Omega_{0}$$
(28a)

$$\mathcal{G}_{c}(d)[\delta d] := \int_{\Omega_{0}} \left\{ \left[ w'(d) + \frac{\eta_{f}}{\tau} \Delta d \right] \delta d + c_{d} \nabla d \cdot \nabla \delta d \right\} d\Omega_{0}$$
(28b)

where the evolution laws (25) have been used to reduce the number of independent fields in the driving energy  $\tilde{\psi}_0$ . The non-local fracture activation functional  $\mathcal{F}_d$  is then defined as:

$$\mathcal{F}_{d}(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^{p},\boldsymbol{\alpha},\boldsymbol{\lambda},d)[\delta d] := \left(\mathcal{G}(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^{p},\boldsymbol{\alpha},\boldsymbol{\lambda},d) - \mathcal{G}_{c}(d)\right)[\delta d]$$
(29)

and condition (22i) is rewritten in the equivalent form

$$\Delta d \ge 0 \quad , \quad \mathcal{F}_d(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \alpha, \lambda, d) \le 0 \quad , \quad \mathcal{F}_d(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \alpha, \lambda, d)[\Delta d] = 0 \tag{30}$$

providing the non-local fracture activation criterion for elastoplastic brittle fracture. It should be noted that in this elastoplastic-brittle-fracture model the only coupling between plastic and fracture dissipation mechanisms is present in the fracture driving force G, while the fracture dissipation  $G_c$  is the same as the one of the purely brittle case.

#### 225 2.4. Constitutive assumptions

For the implementation considered in this work, the general framework described so far is restricted to isotropic linear elastic materials, obeying von Mises plasticity criterion with linear isotropic hardening, i.e.

$$\psi_0^e(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) = \frac{1}{2} K_0 \,\epsilon_v^2 + \frac{1}{2} \, 2G_0 \,(\mathbf{e} - \boldsymbol{\varepsilon}^p) : (\mathbf{e} - \boldsymbol{\varepsilon}^p), \quad f_y(\mathbf{s}_0, \chi_0) = \sqrt{\frac{3}{2} \, \mathbf{s}_0 : \mathbf{s}_0} - \bar{\sigma}_{y0} - \chi_0 \tag{31}$$

where  $K_0$  is the bulk modulus,  $G_0$  is the shear modulus,  $\bar{\sigma}_{y0}$  is the initial yield stress,  $\epsilon_v := \varepsilon : \mathbf{I}$  is the total volumetric strain,  $\mathbf{I}$  being the identity tensor,  $\mathbf{e} = \varepsilon - \frac{1}{3}\epsilon_v \mathbf{I}$  is the deviatoric total strain,  $\mathbf{s}_0 = \sigma_0 - p\mathbf{I}$ , is the deviatoric effective stress, p being the hydrostatic pressure (taken positive if tensile) and  $\chi_0 = H_0 \alpha$  is the static internal variable,  $H_0$  being the hardening modulus. The restriction to von-Mises plasticity allows to identify the internal hardening variable  $\alpha$  with the equivalent plastic strain and its increment is given by  $\Delta \alpha = \sqrt{2/3} \Delta \varepsilon^p : \Delta \varepsilon^p$ .

The phase-field functions  $\omega(d)$  and w(d) are defined as

$$\omega(d) = (1 - d)^2, \quad w(d) = \frac{3G_c}{8l_{0d}}d$$
(32)

where  $G_c$  is the material toughness and  $l_{0d}$  the phase-field internal length. This definition of w(d) corresponds to an AT1 approach, where AT stands for AmbrosioTortorelli and the corresponding type of regularization [43], implying that damage cannot develop until a critical value of the damage driving force has been achieved. Finally, the fracture diffusion coefficient  $c_d$  of the AT1 model is defined as  $c_d = 3/4 G_c l_{0d}$ , the plastic diffusion coefficient  $c_p$  as  $c_p = \sigma_0 l_{0p}^2$ , and the viscous coefficient  $\eta_f$  as  $\eta_f = \bar{\eta} (G_c/l_{0d})$ . To avoid the promotion of crack propagation by predominantly compressive states, the deviatoricvolumetric elastic energy split is adopted (see, e.g. [44, 45]). According to this technique, the elastic energy is split into an *Inactive* part  $\psi_0^{eI}$ , due to negative volumetric strains, and an *Active* remainder  $\psi_0^{eA}$ , which are defined as:

$$\psi_0^{eA}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) = \frac{1}{2} K_0 \langle \boldsymbol{\epsilon}_{\nu} \rangle_+^2 + \frac{1}{2} 2G_0 \left( \boldsymbol{e} - \boldsymbol{\varepsilon}^p \right) : \left( \boldsymbol{e} - \boldsymbol{\varepsilon}^p \right) \qquad , \qquad \psi_0^{eI}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) = \frac{1}{2} K_0 \langle \boldsymbol{\epsilon}_{\nu} \rangle_-^2 \tag{33}$$

where  $\langle \cdot \rangle_{\pm}$  are the Macaulay brackets. In view of the purely deviatoric nature of plastic strains in von Mises plasticity, no distinction is made between the tensile/compressive parts of the plastic component  $\psi^p$  of the free energy density. Note that a split also of this energy component may be recommended in the presence of dilatant elastoplastic materials (see, e.g., [6] for the case of geological materials). The assumed energy split has implications on the definition of the nominal stress and of the plastic dissipation rate. Taking into account the elastic energy split, the nominal free energy is defined as

$$\psi = \omega(\psi_0^{eA} + \psi^p) + \psi_0^{eI}$$
(34)

<sup>250</sup> and, from the dissipation inequality (3), one has that the nominal stress is given by:

$$\boldsymbol{\sigma} = \partial_{\boldsymbol{\varepsilon}^{e}} \boldsymbol{\psi}^{e} = \omega \,\partial_{\boldsymbol{\varepsilon}^{e}} \boldsymbol{\psi}^{eA}_{0} + \partial_{\boldsymbol{\varepsilon}^{e}} \boldsymbol{\psi}^{eI}_{0} = \omega \,\boldsymbol{\sigma}^{A}_{0} + \boldsymbol{\sigma}^{I}_{0} \neq \omega \,\partial_{\boldsymbol{\varepsilon}^{e}} \boldsymbol{\psi}^{e}_{0} = \omega \,\boldsymbol{\sigma}_{0} \tag{35}$$

and no straightforward transformation from effective to nominal stress can be applied. The active and inactive effective stresses are defined:

$$\boldsymbol{\sigma}_{0}^{A} := \partial_{\boldsymbol{\varepsilon}^{e}} \boldsymbol{\psi}_{0}^{eA} \quad , \quad \boldsymbol{\sigma}_{0}^{I} := \partial_{\boldsymbol{\varepsilon}^{e}} \boldsymbol{\psi}_{0}^{eI} \qquad with \qquad \boldsymbol{\sigma}_{0} = \boldsymbol{\sigma}_{0}^{A} + \boldsymbol{\sigma}_{0}^{I} \tag{36}$$

However, for the considered case of von Mises plasticity and volumetric-deviatoric split, one has that  $\sigma_0^I$ :  $\dot{\varepsilon}^p = 0$  and the plastic dissipation rate can still be defined as

$$\dot{\phi} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \chi \dot{\alpha} = \omega \left( \boldsymbol{\sigma}_0^A : \dot{\boldsymbol{\varepsilon}}^p - \chi_0 \dot{\alpha} \right) = \omega \, \dot{\phi}_0 \tag{37}$$

<sup>255</sup> For the case of dilatant geological materials, see also the discussion in [6].

# **3. Modulation of ductile-brittle interaction**

The proposed approach to plasticity-driven phase-field fracture propagation is based on the definition of a non-variational scalar function  $f(\alpha)$  of the equivalent plastic strain, hereafter referred to as *modulation*  *function*, modulating the evolution of the critical fracture energy  $G_c$ , based on the evolution of the plastic process zone. In ductile fracture, the material resistance to crack extension grows due the growth of the plastic zone at the crack tip, until it reaches a limit value (the so-called R-curve). The critical fracture energy  $G_c$  represents this steady state value of the energy to be spent for a unit crack advancement, which however includes also the energy to be dissipated in the creation of the plastic process zone. In the considered model, this latter energy is explicitly taken into account by the plastic dissipation  $\Delta \phi_0^p$ .

To account for these interaction phenomena, the proposed model is based on the assumption that damage, measured by the phase-field order parameter *d*, can grow only when the plastic process zone in a stress concentration region has fully developed, as measured by the local value of the equivalent plastic strain  $\alpha$ . In practical terms, the competition between the plasticity and fracture dissipation mechanisms in the initial crack nucleation phase and their interaction in the subsequent crack propagation phase, is modulated by the addition of a new non-variational interaction term in the expression of the critical energy release rate functional  $\mathcal{G}_c$  (28b):

$$\mathcal{G}_{c}^{\alpha}(\alpha,d)[\delta d] := \underbrace{\int_{\Omega_{0}} f(\alpha) \, w'(d) \, \delta d \, \mathrm{d}\Omega_{0}}_{interaction \ term} + \underbrace{\int_{\Omega_{0}} \left\{ \left[ \, w'(d) + \frac{\eta_{f}}{\tau} \, \Delta d \, \right] \, \delta d + c_{d} \, \nabla d \cdot \nabla \delta d \right\} \, \mathrm{d}\Omega_{0} \qquad (38)$$

The definition of the modulation function  $f(\alpha)$  in (38) is obtained based on the study of the one-dimensional homogeneous case.

It should be noted that the assumed plasticity-driven damage activation criterion, combined with the considered isochoric Mises plasticity model, implies that no damage can develop under a purely hydrostatic tensile stress state. Consideration of this particular failure mode would require an extension of the proposed ductile-brittle interaction model, with a specific treatment of the hydrostatic tensile stress case.

#### 278 3.1. One-dimensional homogeneous case

A one-dimensional problem, with homogeneous distribution of the phase field and of plastic strains, i.e. with  $\nabla d = 0$ ,  $\nabla \Delta \lambda = 0$  and without viscosity, i.e.  $\eta_f = 0$ , is considered. Under these assumptions, the damage activation criterion (30) can be formulated in strong form as follows:

$$\Delta d \ge 0 \quad , \quad -\left[\omega'\left(\psi_0 + \Delta \phi_0^p\right) + (f+1)\frac{3}{8}\frac{G_c}{l_{0d}}\right] \le 0 \quad , \quad \left[\omega'\left(\psi_0 + \Delta \phi_0^p\right) + (f+1)\frac{3}{8}\frac{G_c}{l_{0d}}\right]\Delta d = 0$$

where the definition (32) of the local part w(d) of the phase-field dissipation has been used. Note that, in this simple 1D homogeneous case and thanks to the absence of the gradient of the plastic multiplier, the complementarity condition  $f_y \Delta \lambda = 0$  holds in strong form and, therefore, does not appear in the driving energy (23), which is simply given by  $\tilde{\psi}_0 = \psi_0 + \Delta \phi_0^p$ . When the phase field is evolving, i.e., when  $\Delta d > 0$ , and for  $\omega(d) = (1 - d)^2$ , the activation criterion yields:

$$2(1-d)\left(\psi_0 + \Delta \phi_0^p\right) - (f+1)\frac{3}{8}\frac{G_c}{l_{0d}} = 0$$

where the free energy  $\psi_0$  is defined in (2) and the increment of plastic dissipation  $\Delta \phi_0^p$  in (12). Defining

$$\bar{g} := \frac{3}{16} \frac{G_c}{l_{0d}}$$
(39)

<sup>288</sup> the damage activation condition can be written as:

$$\underbrace{(1-d)\left(\psi_0 + \Delta\phi_0^p\right)}_{driving \ force} \quad -\underbrace{(f+1)\bar{g}}_{effective \ fracture \ energy} = 0 \tag{40}$$

From this equation one can obtain the value of the phase-field variable *d* for prescribed displacement and plastic deformation. The point of view is now reversed. Let us assume that a damage evolution is prescribed, such that damage is zero until a critical value  $\alpha_{cr}$  of the equivalent plastic strain is achieved and that, after this, a fictitious evolution  $\bar{d}(\alpha)$  is prescribed, so that (40) can be solved for  $f(\alpha) + 1$ . For  $\alpha \leq \alpha_{cr}$ ,  $f(\alpha)$ should be a non-decreasing function of the equivalent plastic strain  $\alpha$ , since it is intended to account for the plastic dissipation. As a consequence,  $\psi_0(\alpha)$  in (40) should also be intended as a function that can only increase in time.

To account for all these different aspects, the following form of the modulation function  $f(\alpha)$  has been implemented:

$$f+1 = \begin{cases} f_0 & \text{if} \quad \alpha = 0\\ \frac{\tilde{\mathcal{H}}}{\bar{g}} & \text{if} \quad \alpha \leq \alpha_{cr} \\ (1-\bar{d})\frac{\tilde{\mathcal{H}}}{\bar{g}} + (f_{min}+1)\bar{d} & \text{if} \quad \alpha_{cr} < \alpha < \alpha_{cr} + \Delta\alpha_{cr} \\ f_{min}+1 & \text{if} \quad \alpha_{cr} + \Delta\alpha_{cr} \leq \alpha \end{cases}$$
(41)

where  $f_0$  is an initial value to be defined later and the history function  $\tilde{\mathcal{H}}$  is defined as:

$$\tilde{\mathcal{H}} := \mathcal{H} + \psi_0^p + \Delta \phi_0^p - f_y \Delta \lambda + \frac{1}{2} c_p \nabla \lambda \cdot \nabla \lambda$$
(42)

with the *history variable*  $\mathcal{H}$ , inspired to the one in [46], defined as:

1

$$\mathcal{H} = \max\left(\psi_0^e, \mathcal{H}^n\right) \tag{43}$$

For  $\alpha < \alpha_{cr}$ , this last condition ensures that in the case of elastic unloading, i.e.,  $\psi_0^e < \psi_0^{en}$ , the modulation function cannot decrease. Finally,  $\Delta \alpha_{cr}$  defines the increment of  $\alpha > \alpha_{cr}$  beyond which  $f(\alpha)$  achieves its minimum constant value  $f_{min}$ , corresponding to the purely brittle portion of  $G_c$ , in the sense specified before. According to the definition (41) of  $f(\alpha)$ , after damage activation (i.e., for  $\alpha > \alpha_{cr}$ ) the evolution of  $f(\alpha)$  is governed by the fictitious phase-field history  $\bar{d}(\alpha)$  in (41), whose definition is provided analytically in the form

$$\bar{d}(\alpha) = \begin{cases} 0 & \alpha \le \alpha_{cr} \\ \xi^3 (10 - 15\xi + 6\xi^2) & \alpha_{cr} < \alpha < \alpha_{cr} + \Delta\alpha_{cr} \end{cases} \qquad \xi := \frac{\alpha - \alpha_{cr}}{\Delta\alpha_{cr}}$$
(44)

To better understand the effect of the different parameters in the modulation function  $f(\alpha)$  in (41) and of 306 the prescribed phase-field history  $\bar{d}(\alpha)$  in (44), the proposed ductile-brittle phase-field approach has been 307 applied to a single 4-node element under a uniaxial imposed displacement in plane strain conditions, with 308 the results shown in Figure 2 and 3. The element side is L = 0.01 mm. The element is loaded by  $n_{st} = 100$ 309 equal time steps of imposed vertical displacement  $\Delta u = 0.01 \, mm$ . The used elastoplastic material properties 310 are those shown in Table 1 for Material II. The toughness is changed to the value  $G_c = 100 N/mm$  and the 311 damage internal length is  $l_{0d} = 1 mm$ . Since the element size is much smaller then the plasticity and damage 312 characteristic lengths, the resulting fields will be uniform over the element. The viscous coefficient is set to 313  $\bar{\eta} = 10^{-2}$  s. Three material parameters have been introduced in (41): the critical equivalent plastic strain  $\alpha_{cr}$ , 314 i.e., a scalar measure of the plastic deformation corresponding to the onset of damage; the minimum value 315  $f_{min}$  of the modulation function; the plastic deformation increment  $\Delta \alpha_{cr}$ , beyond which the modulation 316 function  $f(\alpha)$  attains its minimum constant value  $f_{min}$ . Though a precise definition of  $f_{min}$  appears difficult, 317 numerical tests have shown that its influence on the overall response is minor and that it affects mainly the 318 final part of the response curve, when the structure has almost completely failed. In the considered tests, 319  $f_{min} = 0$  has been used obtaining accurate results. It is important to remark that the condition  $\alpha_{cr} > 0$ 320 together with the AT1 assumption ensures the existence of a purely elastoplastic stage before the start of 321 damage. 322



Figure 2: Modulation function  $f(\alpha) + 1$  and fictitious phase-field history  $\bar{d}(\alpha)$ . The model parameters are  $\alpha_{cr} = 0.4$ ,  $\Delta \alpha_{cr} = 0.5$ , and  $f_{min} = 0$ .

The profile of the modulation function  $f(\alpha)$  and of the fictitious phase-field history  $\bar{d}(\alpha)$  are shown in 323 Figure 2. The initial value  $f_0 + 1$  corresponds to the first yielding at the considered material point, i.e., 324 it is given by equation (41) with  $\bar{d} = 0$ ,  $\Delta \phi_0^p = 0$ ,  $\Delta \lambda = 0$  and  $\psi_0$  equal to its value at the yield limit, 325 and therefore is not a model parameter. A very important feature of the proposed form of the modulation 326 function  $f(\alpha)$  is that its evolution is given by the current value of  $\tilde{\mathcal{H}}$  in (41), and does not require to be 327 defined a priori. Therefore, in a multi-dimensional case, for  $\alpha \leq \alpha_{cr}$  the function  $f(\alpha)$  is computed from 328 (41), with  $\bar{d} = 0$ , based on the current values of  $\mathcal{H}$ ,  $\psi_0^p$ ,  $\Delta \phi_0^p$ , and  $\Delta \lambda$ . For  $\alpha \geq \alpha_{cr}$ ,  $\bar{d}$  starts to grow, as 329 specified in (44). At a certain point, the growth of  $\bar{d}$  prevails on the other terms in (41), reducing  $\mathcal{G}_{c}^{\alpha}(\alpha, d)$ 330 in (38), thus allowing damage to propagate. The  $f(\alpha) + 1$  curve reaches a maximum value  $f_{max} + 1$  and then 331 decreases to a minimum value  $f_{min} + 1$ . 332

The effect of the material parameters  $\alpha_{cr}$  and  $\Delta \alpha_{cr}$  is shown in Figure 3 for  $f_{min} = 0$ . The elasto-333 plastic hardening response curve (without damage) is in light gray, while the orange dashed line shows 334 the elastoplastic-brittle response, obtained without the modulation function (i.e. with  $f \equiv 0$ ). It can be 335 clearly noticed how in this latter model there are no parameters to be tuned to better reproduce the material 336 response. In contrast, the introduction of the modulation function allows to achieve the two objectives men-337 tioned before: the competition between the plastic and fracture dissipation mechanisms is modulated by 338 tuning  $\alpha_{cr}$  (Figure 3a), while the interaction between the two mechanisms in the failure phase is modulated 339 by tuning  $\Delta \alpha_{cr}$  (Figure 3b).  $\alpha_{cr}$  delays the beginning of the softening branch, while  $\Delta \alpha_{cr}$  controls its slope. 340

From Figure 3a it appears that  $\alpha_{cr}$  should not be smaller than the value corresponding to the onset of damage in the  $f \equiv 0$  case. The choice of  $f_{min}$  has a minor influence on the response.  $f_{min} = 0$  corresponds to an activation criterion without the effect of the modulation function as in the elastoplastic-brittle case, i.e., the usual value of  $G_c$  is fully recovered in the final phase of the rupture process.



(a) Effects of  $\alpha_{cr}$  on competition between ductile and brittle dissipation mechanisms. For fixed  $\Delta \alpha_{cr} = 0.5$ , the values are  $\alpha_{cr} = 0.2, 0.4, 0.7$ .

(b) Effects of  $\Delta \alpha_{cr}$  on ductile-brittle interaction in failure phase. For fixed  $\alpha_{cr} = 0.4$ , the values are  $\Delta \alpha_{cr} = 0.1, 0.2, 0.5$ .

Figure 3: Effects of modulation function parameters.

## 345 **4. Space discretization**

The problem physical dimension is  $n_{dim}$ , the element number of nodes is  $n_{en}$ , the element number of displacement degrees of freedom is  $n_{ldof} = n_{dim} n_{en}$ . The global number of nodes is  $n_{np}$  and the global number of displacement degrees of freedom is  $n_{dof} = n_{dim} n_{np}$ . The number of independent strain tensor components is  $n_{\varepsilon}$ . The local, elemental and global solutions of the ductile fracture problem can be cast into the column vectors:

$$S_l = (\mathbf{u}, \lambda, d)$$
,  $S_e = (\hat{\mathbf{u}}_e, \hat{\lambda}_e, \hat{\mathbf{d}}_e)$ ,  $S_g = (\hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{d}})$  (45)

where **u** is the displacement vector, of dimensions  $(n_{dim}, 1)$ , while  $\lambda$  is the plastic multiplier and d is the phase field and both are scalar fields. The element nodal displacement vector  $\hat{\mathbf{u}}_e$  has dimensions  $(n_{ldof}, 1)$ , the element multiplier vector  $\hat{\lambda}_e$  has dimensions  $(n_{en}, 1)$  and the element phase-field vector  $\hat{\mathbf{d}}_e$  has dimensions ( $n_{en}$ , 1).  $\hat{\mathbf{u}}$  ( $n_{dof}$ , 1) is the global nodal displacement vector,  $\hat{\lambda}$  ( $n_{np}$ , 1) is the global nodal multiplier vector, and  $\hat{\mathbf{d}}$  ( $n_{np}$ , 1) is the global nodal phase-field vector. The element local solution together with the spatial gradients, i.e. the total deformation  $\boldsymbol{\varepsilon}$  ( $n_{\varepsilon}$ , 1), the plastic multiplier gradient  $\nabla \lambda$  ( $n_{dim}$ , 1) and the phase-field gradient  $\nabla d$  ( $n_{dim}$ , 1) are modeled at the element level as:

$$\mathbf{u} = \mathbf{N}_{\mathrm{u}}\,\hat{\mathbf{u}}_{e} \qquad , \qquad \lambda = \mathbf{N}_{\lambda}\,\hat{\lambda}_{e} \qquad , \qquad d = \mathbf{N}_{\mathrm{d}}\,\hat{\mathbf{d}}_{e} \qquad (46a)$$

$$\boldsymbol{\varepsilon} = \mathbf{B}_{\mathrm{u}} \, \hat{\mathbf{u}}_{e} \qquad , \qquad \boldsymbol{\nabla} \boldsymbol{\lambda} = \mathbf{B}_{\lambda} \, \hat{\boldsymbol{\lambda}}_{e} \qquad , \qquad \boldsymbol{\nabla} d = \mathbf{B}_{\mathrm{d}} \, \hat{\mathbf{d}}_{e}$$
(46b)

where  $\mathbf{N}_{u}$  is the displacement shape function matrix  $(n_{dim}, n_{ldof})$ ,  $\mathbf{B}_{u}$  is displacement compatibility matrix  $(n_{\varepsilon}, n_{ldof})$ ,  $\mathbf{N}_{\lambda}$  and  $\mathbf{N}_{d}$  are the plastic multiplier and phase-field shape function vectors  $(1, n_{en})$ , and  $\mathbf{B}_{\lambda}$  and  $\mathbf{B}_{d}$  are plastic multiplier and phase-field gradient matrices  $(n_{dim}, n_{en})$ . The global assembly is formally performed with the boolean connectivity matrices  $\mathbf{C}_{e,u}$   $(n_{ldof}, n_{dof})$ ,  $\mathbf{C}_{e,\lambda}$   $(n_{en}, n_{np})$ , and  $\mathbf{C}_{e,d}$   $(n_{en}, n_{np})$  such that:

$$\hat{\mathbf{u}}_e = \mathbf{C}_{e,\mathbf{u}}\,\hat{\mathbf{u}} \quad , \qquad \hat{\lambda}_e = \mathbf{C}_{e,\lambda}\,\hat{\lambda} \quad , \qquad \hat{\mathbf{d}}_e = \mathbf{C}_{e,\mathbf{d}}\,\hat{\mathbf{d}}$$
(47)

## 363 4.1. Balance equations

The weak form of the equilibrium equation (22a) and of the plasticity  $(26)_c$  and fracture  $(30)_c$  complementarity equations are spatially discretized:

$$\delta \hat{\mathbf{u}}^{\mathrm{T}} \left[ \sum_{e=1}^{n_{el}} \mathbf{C}_{e,\mathrm{u}}^{\mathrm{T}} \left( \int_{\Omega_{0e}} \mathbf{B}_{\mathrm{u}}^{\mathrm{T}} \boldsymbol{\sigma} \, \mathrm{d}\Omega_{0e} - \int_{\Omega_{0e}} \mathbf{N}_{\mathrm{u}}^{\mathrm{T}} \, \mathbf{b} \, \mathrm{d}\Omega_{0e} - \int_{\partial\Omega_{0e}} \mathbf{N}_{\mathrm{u}}^{\mathrm{T}} \, \mathbf{t} \, \mathrm{d}\Gamma_{e} \right) \right] = 0 \tag{48}$$

366

$$\Delta \hat{\boldsymbol{\lambda}}^{\mathrm{T}} \left[ \sum_{e=1}^{n_{el}} \mathbf{C}_{e,\lambda}^{\mathrm{T}} \left( \int_{\Omega_{0e}} \omega \left[ -\mathbf{N}_{\lambda}^{\mathrm{T}} f_{y} + c_{p} \mathbf{B}_{\lambda}^{\mathrm{T}} \boldsymbol{\nabla} \lambda \right] \mathrm{d}\Omega_{0e} \right) \right] = 0$$
(49)

367

$$\Delta \hat{\mathbf{d}}^{\mathrm{T}} \left[ \sum_{e=1}^{n_{el}} \mathbf{C}_{e,\mathrm{d}}^{\mathrm{T}} \left( \int_{\Omega_{0e}} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \left[ \omega' \,\tilde{\psi}_{0} + (f+1)\,w' + \frac{\eta_{f}}{\Delta t}\,\Delta d \,\right] + c_{d} \,\mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \,\boldsymbol{\nabla} d \right\} \mathrm{d}\Omega_{0e} \right) \right] = 0 \tag{50}$$

where *e* denotes the element number and  $n_{el}$  is the total number of elements in the mesh. The stress tensor in Voigt notation  $\sigma$  is a vector with dimension  $(n_{\sigma}, 1)$ , being  $n_{\sigma} = n_{\varepsilon}$  the number of independent stress components. The element integrals are evaluated over the element nominal volume  $\Omega_{0e}$ . The element internal force vector  $\mathbf{F}_{I,e}$   $(n_{ldof}, 1)$ , the external force vector  $\mathbf{F}_{E,e}$   $(n_{ldof}, 1)$ , the yield vector  $\mathbf{f}_{Y,e}$   $(n_{en}, 1)$ , and <sup>372</sup> the fracture activation vector  $\mathbf{f}_{D,e}$  ( $n_{en}$ , 1) are defined as:

$$\mathbf{F}_{\mathrm{I},e} := \int_{\Omega_{0e}} \mathbf{B}_{\mathrm{u}}^{\mathrm{T}} \left( \omega \, \boldsymbol{\sigma}_{0}^{A} + \boldsymbol{\sigma}_{0}^{I} \right) \mathrm{d}\Omega_{0e}$$
(51a)

$$\mathbf{F}_{\mathrm{E},e} := \int_{\Omega_{0e}} \mathbf{N}_{\mathrm{u}}^{\mathrm{T}} \mathbf{b} \, \mathrm{d}\Omega_{0e} + \int_{\partial\Omega_{0e}} \mathbf{N}_{\mathrm{u}}^{\mathrm{T}} \mathbf{t} \, \mathrm{d}\Gamma_{0e}$$
(51b)

$$\mathbf{f}_{\mathbf{Y},e} := \int_{\Omega_{0e}} \omega \left( \mathbf{N}_{\lambda}^{\mathrm{T}} f_{y} - c_{p} \, \mathbf{B}_{\lambda}^{\mathrm{T}} \, \nabla \lambda \right) \mathrm{d}\Omega_{0e}$$
(51c)

$$\mathbf{f}_{\mathrm{D},e} := -\int_{\Omega_{0e}} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \left[ \omega' \,\tilde{\psi}_{0} + (f+1) \,w' + w'_{\epsilon} + \frac{\eta_{f}}{\Delta t} \,\Delta d \,\right] + c_{d} \,\mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \,\boldsymbol{\nabla} d \right\} \mathrm{d}\Omega_{0e}$$
(51d)

where  $\sigma_0^A$ ,  $\sigma_0^I$  are defined in (36) and  $\nabla \lambda$ ,  $\Delta d$  and  $\nabla d$  are discretized as in (46). The additional constant term  $w'_{\epsilon}$  is introduced to avoid spurious damage activations when  $\alpha < \alpha_{cr}$  and is defined as:

$$w'_{\epsilon} = \epsilon \frac{G_c}{l_{0d}} \operatorname{H}^{-} \left( \alpha - \alpha_{cr} \right)$$
(52)

where  $\epsilon$  is non-dimensional, small coefficient to be set as small as possible (usually taken equal to  $10^{-2}$ ), and H<sup>-</sup> (·) is the negative Heaviside operator. The spatial discretization of the governing equations reads:

$$\mathbf{F}_{\mathrm{I}} - \mathbf{F}_{\mathrm{E}} = \mathbf{0} \tag{53a}$$

$$\Delta \hat{\lambda} \ge \mathbf{0}$$
 ,  $\mathbf{f}_{\mathrm{Y}} \le \mathbf{0}$  ,  $\Delta \hat{\lambda}^{\mathrm{T}} \mathbf{f}_{\mathrm{Y}} = 0$  (53b)

$$\Delta \hat{\mathbf{d}} \ge \mathbf{0} \quad , \quad \mathbf{f}_{\mathrm{D}} \le \mathbf{0} \quad , \quad \Delta \hat{\mathbf{d}}^{\mathrm{T}} \, \mathbf{f}_{\mathrm{D}} = 0$$
 (53c)

# 377 5. Algorithmic implementation

#### 378 5.1. Staggered scheme

The algorithmic solution of the set of governing equations (53) relies on the alternate minimization 379 scheme illustrated in Algorithm 1. At each time step from  $t^n$  to  $t^{n+1}$ , the input is the solution at the previ-380 ous step  $(\hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{d}})_n$ , the increment of displacement Dirichelet boundary conditions  $\Delta \hat{\mathbf{u}}_D$  and the increment of 381 external forces  $\Delta \mathbf{F}_{\rm E}$ . The staggered scheme is solved with an iterative procedure, where *i* denotes the stag-382 gered iteration counter. First, the elastoplastic problem (53a) and (53b) in  $\hat{\mathbf{u}}$  and  $\Delta \hat{\lambda}$  is solved in a monolithic 383 fashion with a Newton-Raphson scheme, for fixed phase-field  $\Delta \hat{\mathbf{d}}_{i-1}$ . The residuum of this inner monolithic 384 loop, with iteration counter k, is a suitable measure of the out-of-balance forces  $\mathbf{F}_{I} - \mathbf{F}_{E}$  and is denoted 385 with  $res_M$ . The corresponding tolerance is  $TOL_M$ , where the M subscript stands for monolithic. Then, the 386 elastoplastic solution  $(\hat{\mathbf{u}}, \hat{\lambda})_k$  is used to solve the phase-field activation criterion for frozen displacement and 387 plastic multiplier. Finally, the residual res<sub>STAG</sub> of the staggered scheme is computed. It measures again 388

the out-of-balance forces, but with the updated damage. The complementarity problems (53b) and (53c) are

solved using the Mangasarian [33] Projected Successive Over-Relaxation algorithm (PSOR), following the

<sup>391</sup> approach proposed in [34]. Further details are given in Appendix C.

Algorithm 1: Alternate minimization scheme

 $(\hat{\mathbf{u}}, \hat{\boldsymbol{\lambda}}, \hat{\mathbf{d}})_{n}, \Delta \hat{\mathbf{u}}_{D}, \Delta \mathbf{F}_{F}$ input initialize  $(\hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{d}})_i = (\hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{d}})_n$ while  $(res_{STAG} > TOL_{STAG})$  do update i = i + 1while  $(res_M > TOL_M)$  do update k = k + 1 $\mathbf{F}_{\mathrm{I},k} = \mathbf{F}_{\mathrm{I}}(\Delta \hat{\mathbf{u}}_{k}, \Delta \hat{\lambda}_{k}, \Delta \hat{\mathbf{d}}_{i-1}) \quad , \quad \mathbf{f}_{\mathrm{Y},k} = \mathbf{f}_{\mathrm{Y}}(\Delta \hat{\mathbf{u}}_{k}, \Delta \hat{\lambda}_{k}, \Delta \hat{\mathbf{d}}_{i-1})$ set  $\begin{aligned} \mathbf{F}_{\mathrm{I},k} - \mathbf{F}_{\mathrm{E}} &= \mathbf{0} \\ \Delta \hat{\boldsymbol{\lambda}}_{k} \geq \mathbf{0} \quad , \quad \mathbf{f}_{\mathrm{Y},k} \leq \mathbf{0} \quad , \quad \Delta \hat{\boldsymbol{\lambda}}_{k}^{\mathrm{T}} \, \mathbf{f}_{\mathrm{Y},k} &= \mathbf{0} \end{aligned} \rightarrow (\Delta \hat{\mathbf{u}}_{k}, \Delta \hat{\boldsymbol{\lambda}}_{k})$ solve assemble  $\mathbf{R}_{\mathrm{u},k} = \mathbf{F}_{\mathrm{I},k}(\Delta \hat{\mathbf{u}}_k, \Delta \hat{\boldsymbol{\lambda}}_k, \Delta \hat{\mathbf{d}}_{i-1}) - \mathbf{F}_{\mathrm{E}}$ compute  $\operatorname{res}_M = \mathbf{R}_{u\,k}^{\mathrm{T}} \mathbf{R}_{u,k}$ end  $(\hat{\mathbf{u}}, \hat{\boldsymbol{\lambda}})_i = (\hat{\mathbf{u}}, \hat{\boldsymbol{\lambda}})_k$ ,  $\mathbf{f}_{\mathrm{D},i} = \mathbf{f}_{\mathrm{D}}(\Delta \hat{\mathbf{u}}_i, \Delta \hat{\boldsymbol{\lambda}}_i, \Delta \hat{\mathbf{d}})$ set  $\Delta \hat{\mathbf{d}} \ge \mathbf{0}$  ,  $\mathbf{f}_{\mathrm{D},i} \le \mathbf{0}$  ,  $\Delta \hat{\mathbf{d}}^{\mathrm{T}} \mathbf{f}_{\mathrm{D},i} = 0 \longrightarrow \Delta \hat{\mathbf{d}}_{i} = \Delta \hat{\mathbf{d}}$ solve assemble  $\mathbf{R}_{u,i} = \mathbf{F}_{I}(\Delta \hat{\mathbf{u}}_{i}, \Delta \hat{\lambda}_{i}, \Delta \hat{\mathbf{d}}_{i}) - \mathbf{F}_{E}$  $\operatorname{res}_{STAG} = \mathbf{R}_{\mathrm{u},i}^T \mathbf{R}_{\mathrm{u},i}$ compute end output  $(\hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{d}})_n = (\hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{d}})_i$ 

#### 392 5.2. Monolithic elastoplastic solver

The solution scheme of the elastoplastic problem (53a) and (53b) is further detailed in this section. Since in the light of the staggered scheme this problem must be solved for fixed phase-field, the explicit dependence on the damage variable is omitted for the sake of clarity. The displacement residual vector  $\mathbf{R}_{u}$ (the iteration conter *k* has been omitted for notation convenience) has dimensions ( $n_{dof}$ , 1) and measures the <sup>397</sup> out-of-balance forces in the equilibrium equations:

$$\mathbf{R}_{\mathrm{u}}(\Delta \hat{\mathbf{u}}, \Delta \hat{\boldsymbol{\lambda}}) := \mathbf{F}_{\mathrm{I}}(\Delta \hat{\mathbf{u}}, \Delta \hat{\boldsymbol{\lambda}}) - \mathbf{F}_{\mathrm{E}}$$
(54)

The solution of the balance of linear momentum must fulfill the elastoplastic laws (53b). In practical terms, the loading-unloading conditions (53b) must be solved for fixed displacement increment, with the additional difficulty that, due to the presence of the gradient term, the elastoplastic return mapping algorithm has to be formulated as a global problem and the time integration of the constitutive law cannot be carried out element by element. Once a first estimate of the nodal plastic multiplier increment  $\Delta \hat{\lambda}$  is obtained, the set of active nodes  $\mathcal{A}$  can be determined using the global PSOR algorithm:

$$\mathcal{A} := \left\{ a \in [1, n_{np}] \mid \Delta \hat{\lambda}_a > 0 \right\}$$
(55)

where *a* is the global node label. The vanishing of the residuum  $\mathbf{R}_{u}$  is enforced by means of a Newton-Raphson iterative scheme. The estimate of the displacement increment update  $\delta \Delta \hat{\mathbf{u}}$  between two successive iteration k - 1 and k can be computed from the following conditions, resulting from the linearization of  $\mathbf{R}_{u}$ and  $\mathbf{f}_{Y}$  around the current solution  $\hat{\mathbf{u}}_{k-1}$ ,  $\Delta \hat{\lambda}_{k-1}$ :

$$\delta \mathbf{R}_{u} + \mathbf{R}_{u} = \mathbf{0} \quad , \quad \delta \mathbf{f}_{Y} \Big|_{\mathcal{H}} = \mathbf{0} \tag{56}$$

where  $(\cdot)|_{\mathcal{R}}$  is the restriction over the set of active nodes. The linearizations read:

$$\delta \mathbf{R}_{\mathrm{u}} = \frac{\partial \mathbf{R}_{\mathrm{u}}}{\partial \hat{\mathbf{u}}} \,\delta \Delta \hat{\mathbf{u}} + \frac{\partial \mathbf{R}_{\mathrm{u}}}{\partial \hat{\lambda}} \Big|_{\mathcal{A}} \,\delta \Delta \hat{\boldsymbol{\lambda}} \Big|_{\mathcal{A}} = \mathbf{K}_{\mathrm{uu}} \,\delta \Delta \hat{\mathbf{u}} + \mathbf{K}_{\mathrm{u\lambda}} \Big|_{\mathcal{A}} \,\delta \Delta \hat{\boldsymbol{\lambda}} \Big|_{\mathcal{A}} \tag{57a}$$

$$\delta \mathbf{f}_{\mathrm{Y}} = \frac{\partial \mathbf{f}_{\mathrm{Y}}}{\partial \hat{\mathbf{u}}} \bigg|_{\mathcal{A}} \delta \Delta \hat{\mathbf{u}} + \frac{\partial \mathbf{f}_{\mathrm{Y}}}{\partial \hat{\lambda}} \bigg|_{\mathcal{A}} \delta \Delta \hat{\boldsymbol{\lambda}} \bigg|_{\mathcal{A}} = \mathbf{K}_{\lambda u} \, \delta \Delta \hat{\mathbf{u}} + \mathbf{K}_{\lambda \lambda} \bigg|_{\mathcal{A}} \, \delta \Delta \hat{\boldsymbol{\lambda}} \bigg|_{\mathcal{A}}$$
(57b)

<sup>409</sup> Therefore, the solving system becomes:

$$\begin{bmatrix} \mathbf{K}_{\mathrm{uu}} & \mathbf{K}_{\mathrm{u\lambda}} |_{\mathcal{A}} \\ \mathbf{K}_{\mathrm{\lambda}\mathrm{u}} |_{\mathcal{A}} & \mathbf{K}_{\mathrm{\lambda}\mathrm{\lambda}} |_{\mathcal{A}} \end{bmatrix}_{k-1} \begin{vmatrix} \delta \Delta \hat{\mathbf{u}} \\ \delta \Delta \hat{\boldsymbol{\lambda}} |_{\mathcal{A}} \end{vmatrix} = - \begin{vmatrix} \mathbf{R}_{\mathrm{u}} \\ \mathbf{0} \end{vmatrix}_{k-1}$$
(58)

It is important to remark that this system is needed only to recover the correct algorithmic tangent stiffness 410 for the estimation of the displacement update  $\delta \Delta \hat{\mathbf{u}}$  through (57a). Once the system has been solved for  $\delta \Delta \hat{\mathbf{u}}$ , 411 the value of the update  $\delta \Delta \hat{\lambda} \Big|_{\mathcal{A}}$  is not used in the current algorithm. As shown in Algorithm 2, it is evident 412 how the adopted procedure resembles a classical Newton-Raphson scheme for local plasticity, but with the 413 introduction of a global return mapping. The explicit expressions of the tangent matrix and residuals are 414 provided in Appendix A. When large time steps are used, convergence may become difficult. especially 415 when damage is activated. To overcome convergence problems, a line search procedure has been used as 416 outlined in Appendix B. 417

while  $(res_M > TOL_M)$  do assemble  $\mathbf{K}_{uu}(\Delta \hat{\mathbf{u}}_k, \Delta \hat{\lambda}_k)$ ,  $\mathbf{K}_{u\lambda}(\Delta \hat{\mathbf{u}}_k)$ ,  $\mathbf{K}_{\lambda\lambda}$ k = k + 1update  $\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\lambda} |_{\mathcal{A}} \\ \mathbf{K}_{\lambda u} |_{\mathcal{A}} & \mathbf{K}_{\lambda \lambda} |_{\mathcal{A}} \end{bmatrix}_{k-1} \begin{vmatrix} \delta \Delta \hat{\mathbf{u}} \\ \delta \Delta \hat{\boldsymbol{\lambda}} |_{\mathcal{A}} \end{vmatrix} = - \begin{vmatrix} \mathbf{R}_{u} \\ \mathbf{0} \end{vmatrix}_{k-1} \rightarrow \Delta \hat{\mathbf{u}}_{k} = \Delta \hat{\mathbf{u}}_{k-1} + \delta \Delta \hat{\mathbf{u}}$ solve  $\mathbf{f}_{\mathbf{Y},k} = \mathbf{f}_{\mathbf{Y}}(\Delta \hat{\mathbf{u}}_k, \Delta \hat{\boldsymbol{\lambda}})$ set  $\Delta \hat{\lambda} \ge \mathbf{0}$  ,  $\mathbf{f}_{\mathbf{Y},k} \le \mathbf{0}$  ,  $\Delta \hat{\lambda}^{\mathrm{T}} \mathbf{f}_{\mathbf{Y},k} = 0 \longrightarrow \Delta \hat{\lambda}_{k} = \Delta \hat{\lambda}$ solve  $\mathcal{A} := \{ a \in [1, n_{np}] \mid \Delta \hat{\lambda}_{k,a} > 0 \}$ define assemble  $\mathbf{R}_{u,k}(\Delta \hat{\mathbf{u}}_k, \Delta \hat{\boldsymbol{\lambda}}_k)$  $\texttt{res}_M = \mathbf{R}_{\mathrm{u},k}^T \, \mathbf{R}_{\mathrm{u},k}$ compute end

#### 418 **6. Numerical simulations**

Two-dimensional simulations are performed with 4-nodes quadrilateral elements in plane strain condi-419 tions. One of the consequences of the effective stress approach is that plastic strains continue to develop until 420 the final stage of failure, therefore requiring a suitable treatment of plastic locking. Here, a reduced one-421 point integration rule with hourglass control has been used for all fields  $\mathbf{u}, \lambda, d$ , in line with what proposed 422 in [47]. The staggered residual tolerance is  $TOL_{STAG} = 10^{-3} N^2$ , while the monolithic Newton-Raphson 423 residual tolerance is  $TOL_M = 10^{-6} N^2$ . The mesh resolution of the phase-field localization band is reported 424 for each test comparing the element dimension  $h_e$  and the damage internal length parameter  $l_{0d}$ , which for 425 the AT1 dissipation model represents a fourth of the band width (see e.g. [48]). 426

Material	$E_0$	ν	$K_0$	$G_0$	$\sigma_0$	$H_0$	$l_{0p}$	$G_c$
Ι	68.90	0.33	-	-	465	10	1.2	10
II	-	-	71.66	27.28	340	250	1.6	9.31
	GPa	-	GPa	GPa	MPa	MPa	mm	N/mm

Table 1: Material properties

#### 427 6.1. One-dimensional localization

The tensile loading of a one-dimensional bar is considered. The geometry and boundary conditions are depicted in Figure 4. The cross section is assumed to be  $A = 1 mm^2$ . The material properties are  $E_0 = 210 GPa$ ,  $\sigma_0 = 350 MPa$ ,  $H_0 = 650 MPa$ ,  $l_{0p} = 0.06 mm$ , and  $G_c = 2 N/mm$ . The fracture internal length is  $l_{0d} = 0.03 mm$ . The ductile fracture parameters are  $\alpha_{cr} = 0.4$ ,  $\Delta \alpha_{cr} = 0.2$  and  $f_{min} = 0$ . The viscous coefficient  $\bar{\eta} = 5 \cdot 10^{-3} s$ .

A uniform mesh of 500 linear one-dimensional finite elements is used with an element size  $h_e =$ 0.002 mm. A uniform time discretization is used to enforce the boundary conditions. The total number of steps is  $n_{st} = 1000$  and the step increment is  $\Delta \bar{u} = 5 \cdot 10^{-4}$  mm. The localization in the central part of the bar is obtained with a local weakening of the material properties in the central 10% of its length. In these elements, the yield stress  $\sigma_0$  and the toughness  $G_c$  are reduced by 20%. For this particular 1D example, the staggered residual tolerance is TOL<sub>STAG</sub> =  $10^{-5}$  N<sup>2</sup>, while the monolithic Newton-Raphson residual tolerance is TOL<sub>M</sub> =  $10^{-10}$  N<sup>2</sup>.



Figure 4: One-dimensional bar in tension: geometry [mm] and boundary conditions.

The global response in terms of engineering strain and stress is shown in Figure 5a. Here, some significant steps are highlighted with circular markers. The corresponding profiles of the modulation function f + 1 are then plotted in Figure 5b. The first time at which a point reaches  $\alpha = \alpha_{cr}$  is step 680. The competition between the terms  $(1 - \bar{d})$  and  $\tilde{H}$  starts at step 737. Until that moment, the qualitative profile of the modulation function resembles the one of the equivalent plastic deformation. After that, the points experiencing a plastic deformation  $\alpha > \alpha_{cr}$  show a decrease in the value of f + 1, since the influence of the fictitious phase-field history  $\bar{d}$  significantly intervenes into the modulation function.



Figure 5: 1D localization. Global response (a) and modulation function time evolution (different colors correspond to different times) (b).

The time and space evolution of the equivalent plastic deformation and of the phase field can be observed 447 in Figure 6. The circular markers correspond to the mesh nodes. Before damage onset, only the plastic 448 deformation profile is different from zero as shown in the plot of step 680, when for the first time  $\alpha = \alpha_{cr}$ 449 is reached. Here, the uniform solution of the equivalent plastic deformation is slightly perturbed by the 450 weakening of the material parameters. In the following steps, the damage localization induces a more 451 intense localization of plastic deformations, due to the effective stress approach adopted in the current 452 work, with the material continuing to yield after damage development. Since the effective stress is acting on 453 the continuous part of the material bulk and this is progressively reducing, the plastic deformation increases 454 considerably and, at this point, the effect of the gradient on the plastic multiplier can be appreciated because 455 of the softening structural response. In the subsequent snapshots, it can be noticed how the damage growth 456 is driven by the developing plastic strain. At step 752, the plastic deformation reaches  $\alpha_{cr} + \Delta \alpha_{cr}$  for the 457 first time. At step 800, the profiles of the equivalent plastic deformation and of the phase field are fully 458 developed. The plasticity driven nature of fracture can be appreciated by noticing that the finite band-width 459 of damage is entirely contained in the plastic localization band, since no damage occurs in the portion of 460 the domain where  $\alpha < \alpha_{cr}$ . 461



Figure 6: 1D localization. Equivalent plastic strain (blue curve) and phase-field time evolution (brown curve).

#### 462 6.2. V-notched specimen

We consider the V-notched specimen experimentally tested in [49]. Several authors have used this benchmark for the simulation of ductile fracture (see, e.g., [19]). This is shown as a first example to demonstrate the model capabilities when crack onset and specimen failure occur without a stable propagation branch. The geometry of the specimen is depicted in Figure 7a. As in [49, 19], slightly rounded corners have been used at the notch tips to avoid sharp discontinuities in the geometry. The Dirichelet boundary conditions constrain the horizontal direction only. The material properties are shown in Table 1 for the case of Material I. The phase-field internal length is  $l_{0d} = 0.4 mm$  and the ductile fracture parameters are  $\alpha_{cr} = 0.05$ ,  $\Delta \alpha_{cr} = 0.03$  and  $f_{min} = 0$ .



(b) Mesh

Figure 7: V-notched specimen. Geometry in [mm], boundary conditions and mesh.

- <sup>471</sup> The mesh is shown in Figure 7b. A refinement in the expected crack propagation region is used. The
- <sup>472</sup> minimum element side is  $h_e = 0.1 \text{ mm}$ . The resolution of the localization zone is  $l_{0p}/h_e = 12$  for the plastic
- <sup>473</sup> deformation and  $l_{od}/h_e = 4$  for the phase field. A total of  $n_{el} = 6359$  elements and  $n_{np} = 6454$  nodes have
- <sup>474</sup> been used, with a time step  $\Delta u = 0.01 mm$ .



Figure 8: V-notched specimen. Reaction force vs imposed displacement. Results (solid black curve) are compared to those in [19] (light gray) and to the experimental results in [49] (circular markers).

The global response in terms of reaction force and enforced displacement at the right edge is shown in 475 Figure 8. The viscous coefficient is set to a non-negligible value  $\bar{\eta} = 0.08 s$ , to prevent overly brittle crack 476 propagation. The response is purely elastoplastic until a displacement of 0.25 mm, corresponding to step 477 25, is enforced. Then, damage grows at both the notch tips until crack onset occurs between step 35 and 478 36. The two cracks propagate with an almost linear path until step 42, when the first crack starts to branch 479 as it can be clearly noticed in step 44. The final coalescence of the two fractures occurs at step 49. The 480 contour plots of the plastic multiplier  $\lambda$  and of the phase field d at the relevant steps in the reaction curve 481 are shown in Figure 9. It must be noticed that, due to the plasticity driven nature of the proposed ductile 482 fracture model, the crack propagation closely follows the path of the plasticity localization band observable 483 in the contour plots of  $\lambda$ . 484



Figure 9: V-notched specimen. Plastic multiplier and phase-field contourplots.

# 485 6.3. Symmetric notched specimen

This test has also been investigated by several authors, such as in [4] and [9]. In these two works, the ductile fracture simulation approach is significantly different from the current model. The main difference lies in the yield criterion being based on nominal stresses. When damage starts to propagate, nominal stresses decrease and the response of the damaged material becomes purely elastic, since the yield surface can be no more activated. This example is particularly interesting in view of the stable crack propagation that can be observed after damage reaches the unit value in the first notch. The geometry and boundary conditions are shown in Figure 10a. Both edges are clamped (i.e, no horizontal displacements are allowed) and the top boundary is subjected to an enforced vertical displacement. The uniform increment of Dirichelet boundary conditions at each step is  $\Delta u = 0.01 \text{ mm}$ .



Figure 10: Symmetric notched specimen. Geometry in [mm], boundary conditions (a) and mesh (b).

The material properties are shown in Table 1 for the case of Material II. The phase-field internal length is  $l_{0d} = 0.4 mm$  and the ductile fracture parameters are  $\alpha_{cr} = 0.09$ ,  $\Delta \alpha_{cr} = 0.01$  and  $f_{min} = 0$ . The viscous coefficient is  $\bar{\eta} = 0.01 s$ . The mesh for the simulation is shown in Figure 10b. A local refinement is introduced where the crack propagation is expected to occur. The minimum element side is  $h_e = 0.2 mm$ . The resolution of the localization zone is  $l_{0p}/h_e = 8$  for the plastic deformation and  $l_{0d}/h_e = 2$  for the phase field. The number of elements is  $n_{el} = 5438$  and the number of nodes is  $n_{np} = 5494$ .



Figure 11: Symmetric notched specimen. Reaction force vs imposed displacement. Results are compared with those of the nominal stress approach proposed in Ambati et al [4].

The global response in terms of reaction force vs enforced vertical displacement at the top edge is depicted 501 in Figure 11. The corresponding contour plots of plastic multiplier and phase field are shown in Figure 12. 502 The response is purely elastoplastic until step 55 corresponding to  $\bar{u} = 0.55 \text{ mm}$ . In step 71 it is evident how 503 shear bands form at an inclination of almost 45°. At step 80 ( $\bar{u} = 0.80 \, mm$ ), the right notch first reaches 504 damage equal to unity. Afterwards, a long and stable horizontal crack propagation is observed from the right 505 notch towards the opposite one. This mechanism continues until step 113 ( $\bar{u} = 1.13 \text{ mm}$ ) with an almost 506 linear softening slope. At this point the crack in the second notch appears. Then, in a few steps, a short 507 stable propagation of this second crack is observed towards the opposite side. This mechanism is evident up 508 to step 148 ( $\bar{u} = 1.48 \text{ mm}$ ) when the cracks are so close that the merging of the two paths becomes possible. 509 This sudden crack propagation ends with the specimen failure at step 153 ( $\bar{u} = 1.53 \text{ mm}$ ). 510



0.14 0.21 0.28

0

0.07

(a) Plastic multiplier  $\lambda$ 

#### $0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1$



(b) Phase field d

Figure 12: Symmetric notched specimen. Plastic multiplier (a) and phase field (b) contour plots.

# 511 6.4. Asymmetric notched specimen

The asymmetric notched specimen with the geometry and boundary conditions depicted in Fig. 13a is considered. The bottom edge is fully clamped, while the top edge has fully constrained horizontal displacement, with an enforced vertical displacement  $\bar{u}$ . The material properties correspond to Material I in Table 1. The phase-field internal length is  $l_{0d} = 0.6 mm$  and the ductile fracture parameters are  $\alpha_{cr} = 0.086$ ,  $\Delta \alpha_{cr} = 0.05$  and  $f_{min} = 0$ . The viscous coefficient is  $\bar{\eta} = 0.001 s$ .



Figure 13: Asymmetric notched specimen. Geometry in [mm], boundary conditions (a) and mesh (b).

The mesh used is shown in Figure 13b. The spatial discretization is locally refined where the crack localization is expected to occur. The minimum element size is  $h_e = 0.2 \text{ mm}$ . Therefore, the resolution is  $l_{0p}/h_e = 8$ and  $l_{0d}/h_e = 3$ . The number of elements is  $n_{el} = 2637$  and the number of nodes is  $n_{np} = 2686$ . The time step is  $\Delta u = 0.01 \text{ mm}$ .



Figure 14: Asymmetric notched specimen. Reaction force vs imposed displacement. Results are compared with those obtained with the nominal stress approach proposed in Ambati et al [4] and the effective stress approach proposed in Rodriguez et al [11].

The global response in terms of reaction force and enforced displacement is shown in Figure 14. The structural response is elastoplastic until step 45 where a damage starts to develope at the upper notch. At step 61, the phase-field reaches unity for the first time. At step 64, fracture starts also from the lower notch. First, the cracks propagate horizontally from the two notches, then, in few steps, the two paths start to align along the shear band, i.e., in the direction of the driving plastic deformation. Finally, an unstable crack propagation occurs between steps 79 and 81, where the cracks merge.



(a) Plastic multiplier  $\lambda$ 





(b) Phase field d

Figure 15: Asymmetric notched specimen. Contour plots of plastic multiplier (a) and phase field (b).

## 527 7. Conclusions

A variational formulation of small strain ductile fracture, based on an AT1 phase-field modeling of crack propagation, has been proposed. The main features of the proposed model can be summarized as follows.

• A mixed variational statement has been formulated, incorporating a finite-step variational update for both gradient elastoplasticity and the phase field. The obtained functional is of a general form and can be used for any elastoplastic model belonging to the class of generalized standard materials [38].

- Irreversibility of both plastic and brittle dissipation has been enforced in a rigorous way formulating
   the two problems as global linear complementarity problems. Both problems have been solved using
   a very efficient explicit Projected Successive Over-Relaxation (PSOR) algorithm [33], following the
   approach proposed in [32, 34].
- The elastoplastic model has been formulated in terms of effective stresses, i.e. the true stresses acting 537 on the non-damaged part of the bulk material. This has at least two important consequences. First, 538 available implementations of elastoplastic models need not be modified and can be directly used as 539 they are. This is of particular interest, e.g., in the case of anisotropic materials. Second, while in the 540 case of nominal stresses plastic strains stop to grow as soon as damage starts to develop, in the case 541 of effective stresses, plasticity continues to develop until the very final stage of rupture, making the 542 gradient plasticity regularization necessary and also requiring a dedicated treatment of elastoplastic 543 locking. 544
- In ductile fracture, damage growth is associated to locally high levels of plastic strains. A plasticity 545 driven crack propagation model has therefore been formulated. The complex interaction between 546 ductile and brittle dissipation has been modulated by the addition of a non-variational function of 547 the equivalent plastic strain, in the line of what proposed by several other authors [4, 7, 9, 17]. The 548 adopted modulation function depends on three parameters whose role is clearly identified and which 549 can be easily determined based on a one-dimensional tension test. Another important feature, is that 550 until a critical value of the equivalent plastic strain is achieved, the value of the modulation function 551 is determined directly by the structural response and need not be established a priori, conferring great 552 generality to its definition. 553
- A staggered algorithm has been formulated for the solution of the variational equations. The gradient elastoplastic problem is solved monolithically for fixed phase field, while the phase-field problem is

solved for fixed displacements and plastic strains. The monolithic solution of the gradient elasto plastic problem is often critical and requires special attention. A consistent global Newton-Raphson
 scheme has been formulated for the case of Mises plasticity, with a return mapping carried out at
 global level, together with a rigorous consistent tangent matrix. The convergence has been further
 improved supplementing the iterative scheme with a line-search procedure.

The proposed model has been applied to the simulation of several benchmark problems revealing excellent robustness, good accuracy and easy parameter identification. Extension to 3D finite strain ductile fracture is currently in progress.

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# 568 Appendix A. Linearizations for isotropic von-Mises gradient elastoplasticity

The linearizations needed for the solution of the gradient elastoplastic problem with the monolithic scheme in Algorithm 2 are developed below. All operations are performed for the gradient Mises elastoplastic problem without damage and the zero subscript of the effective response is omitted for the sake of clarity. Voigt notation is used throughout this appendix. For instance, the stress vector is denoted with  $\sigma$ . The linearization of the element internal forces vector reads:

$$\delta \mathbf{F}_{\mathbf{I},e} = \int_{\Omega_{e}} \mathbf{B}_{\mathbf{u}}^{\mathrm{T}} \, \delta \boldsymbol{\sigma} \, \mathrm{d}\Omega_{e} = \underbrace{\left[ \int_{\Omega_{e}} \mathbf{B}_{\mathbf{u}}^{\mathrm{T}} \left( \mathbf{D}^{el} - \Delta \lambda \, \mathbf{D}_{dev}^{el} \, \partial_{\boldsymbol{\sigma}\boldsymbol{\sigma}}^{2} f_{y} \, \mathbf{D}_{dev}^{el} \right) \mathbf{B}_{\mathbf{u}} \, \mathrm{d}\Omega_{e} \right]}_{\mathbf{K}_{uu,e}} \delta \hat{\mathbf{u}}_{e} + \underbrace{\left[ \int_{\Omega_{e}} \mathbf{B}_{\mathbf{u}}^{\mathrm{T}} \left( - \mathbf{D}_{dev}^{el} \, \partial_{\boldsymbol{\sigma}} f_{y} \right) \mathbf{N}_{\lambda} \, \mathrm{d}\Omega_{e} \right]}_{\mathbf{K}_{u\lambda,e}} \delta \hat{\lambda}_{e}$$
(A.1)

where  $\mathbf{D}^{el} = \partial_{\varepsilon\varepsilon}^2 \psi^e$  is the matrix of elastic moduli and the deviatoric nature of the plastic deformation vector  $\mathbf{\epsilon}^p$  has been exploited.  $\mathbf{D}_{dev}^{el}$  is the deviatoric elastic stiffness matrix. The linearization of the element yield 576 vector reads:

579

$$\delta \mathbf{f}_{\mathbf{Y},e} = \int_{\Omega_{e}} \left[ \mathbf{N}_{\lambda}^{\mathrm{T}} \, \delta f_{y} - c_{p} \, \mathbf{B}_{\lambda}^{\mathrm{T}} \, \boldsymbol{\nabla} \delta \lambda \right] \mathrm{d}\Omega_{e} = \\ = \left[ \int_{\Omega_{e}} \mathbf{N}_{\lambda}^{\mathrm{T}} \left( \mathbf{D}_{dev}^{el} \, \partial_{\sigma} f_{y} \right)^{\mathrm{T}} \mathbf{B}_{\mathrm{u}} \, \mathrm{d}\Omega_{e} \right] \delta \hat{\mathbf{u}}_{e} + \\ \frac{\mathbf{K}_{\lambda \mathrm{u},e}}{\mathbf{K}_{\lambda}} \left[ \int_{\Omega_{e}} \left\{ \mathbf{N}_{\lambda}^{\mathrm{T}} \left( \partial_{\sigma} f_{y}^{\mathrm{T}} \, \mathbf{D}_{dev}^{el} \, \partial_{\sigma} f_{y} + \partial_{\lambda} \chi \right) \mathbf{N}_{\lambda} + c_{p} \, \mathbf{B}_{\lambda}^{\mathrm{T}} \, \mathbf{B}_{\lambda} \right\} \mathrm{d}\Omega_{e} \right] \delta \hat{\boldsymbol{\lambda}}_{e}$$

$$(A.2)$$

The deviatoric elastic stiffness matrix for the isotropic case is  $\mathbf{D}_{dev}^{el} = 2G \mathbf{I}_{dev}$ , where  $\mathbf{I}_{dev}$  is the deviatoric projection matrix. The use of von-Mises yield function with isotropic linear hardening leads to:

$$\Delta \lambda \mathbf{D}_{dev}^{el} \partial_{\sigma\sigma}^{2} f_{y} \mathbf{D}_{dev}^{el} = 2G\beta \left( \mathbf{I}_{dev} - \mathbf{n}^{tr} \mathbf{n}^{trT} \right)$$
$$\mathbf{D}_{dev}^{el} \partial_{\sigma} f_{y} = 3G \frac{\mathbf{s}^{tr}}{\sigma_{eq}^{tr}} \quad , \quad \partial_{\sigma} f_{y}^{T} \mathbf{D}_{dev}^{el} \partial_{\sigma} f_{y} = 3G$$

where  $\mathbf{s}^{tr}$  is the trial elastic deviatoric stress vector,  $\mathbf{n}^{tr} = \mathbf{s}^{tr}/|\mathbf{s}^{tr}|$  is the trial yield surface unit normal vector,  $\sigma_{eq}^{tr} = \sqrt{3/2} \, \mathbf{s}^{tr} : \mathbf{s}^{tr}$  is the trial equivalent stress (being **s** the deviatoric stress tensor with Voigt notation **s**), and  $\beta := {}^{3G} \Delta \lambda / \sigma_{eq}^{tr}$ . The element tangent stiffness matrices and the internal forces vector are:

$$\mathbf{K}_{\mathrm{uu},e} = \int_{\Omega_e} \mathbf{B}_{\mathrm{u}}^{\mathrm{T}} \left[ \mathbf{D}^{el} - 2G\beta \left( \mathbf{I}_{dev} - \mathbf{n}^{tr} \mathbf{n}^{tr\mathrm{T}} \right) \right] \mathbf{B}_{\mathrm{u}} \, \mathrm{d}\Omega_e \tag{A.3a}$$

$$\mathbf{K}_{\boldsymbol{u}\boldsymbol{\lambda},e} = \int_{\Omega_e} \mathbf{B}_{\boldsymbol{u}}^{\mathrm{T}} \left( -3G \, \frac{\mathbf{s}^{tr}}{\sigma_{eq}^{tr}} \right) \mathbf{N}_{\boldsymbol{\lambda}} \, \mathrm{d}\Omega_e = \mathbf{K}_{\boldsymbol{\lambda}\boldsymbol{u},e}^{\mathrm{T}}$$
(A.3b)

$$\mathbf{K}_{\lambda\lambda,e} = -\int_{\Omega_e} \left[ \left( 3G + H \right) \mathbf{N}_{\lambda}^{\mathrm{T}} \mathbf{N}_{\lambda} + c_p \, \mathbf{B}_{\lambda}^{\mathrm{T}} \, \mathbf{B}_{\lambda} \right] \mathrm{d}\Omega_e \tag{A.3c}$$

$$\mathbf{F}_{\mathbf{I},e} = \int_{\Omega_e} \mathbf{B}_{\mathbf{u}}^{\mathrm{T}} \left[ p \,\mathbf{1} + (1-\beta) \,\mathbf{s}^{tr} \right] \mathrm{d}\Omega_e \tag{A.3d}$$

<sup>583</sup> where **1** is the spherical projection vector in Voigt notation.

# 584 Appendix B. Steepest descent or backtracking line search

The implemented line search procedure is based on what proposed in [50]. The global return mapping outlined in Section 5.2 for the elastoplastic gradient problem with fixed damage shows how the loadingunloading condition (53b) is a purely displacement driven problem. Therefore, without loss of generality, it can be stated that the total energy is a function of displacement only  $\Pi_p^{\nabla n}(\Delta \hat{\mathbf{u}})$ . The solution update  $\delta \Delta \hat{\mathbf{u}}$  between two subsequent Newton iterations k - 1 and k is the result of the monolithic system (58) and the current solution can be written as follows:

$$\Delta \hat{\mathbf{u}}_k = \Delta \hat{\mathbf{u}}_{k-1} + \delta \Delta \hat{\mathbf{u}} \tag{B.1}$$

The new solution estimate should satisfy the condition  $\Pi_p^{\nabla n}(\Delta \hat{\mathbf{u}}_k) < \Pi_p^{\nabla n}(\Delta \hat{\mathbf{u}}_{k-1})$ . Yet, this condition may not be always fullfiled by the Newton algorithm. Therefore, a line search procedure has been implemented. The step length parameter  $\gamma_k$  is defined such that:

$$\Delta \hat{\mathbf{u}}_k = \Delta \hat{\mathbf{u}}_{k-1} + \gamma_k \,\,\delta \Delta \hat{\mathbf{u}} \tag{B.2}$$

<sup>594</sup> The optimal step length minimizes the total energy between the two iterations k - 1 and k:

$$\gamma_k = \arg\min_{\gamma_k^*} \left[ \Pi_p^{\nabla n} \left( \Delta \hat{\mathbf{u}}_{k-1} + \gamma_k^* \, \delta \Delta \hat{\mathbf{u}}_k \right) \right] \tag{B.3}$$

For non-quadratic objective functions  $\Pi(\Delta \hat{\mathbf{u}})$  there is no closed form solution of the problem (B.3). Therefore, a standard procedure involves the satisfaction of the so-called Wolfe condition:

$$\Pi_{p}^{\nabla n}(\Delta \hat{\mathbf{u}}_{k-1} + \gamma_k \,\delta \Delta \hat{\mathbf{u}}_k) < \Pi_{p}^{\nabla n}(\Delta \hat{\mathbf{u}}_{k-1}) + c_1 \,\gamma_k \,\delta \Delta \hat{\mathbf{u}}_k^{\mathrm{T}} \,\mathbf{R}_{\mathrm{u}}(\Delta \hat{\mathbf{u}}_{k-1}) \tag{B.4}$$

where  $\mathbf{R}_{u}$  is the global displacement residual vector defined in (54) and  $\mathbf{R}_{u}(\Delta \hat{\mathbf{u}}_{k-1})$  is the residual at the previous iteration used for the computation of  $\delta \Delta \hat{\mathbf{u}}_{k}$ . The constant parameter  $c_{1}$  for Newton type solver has the typical value  $10^{-4}$  (see [50]).

Algorithm 3: Backtracking or steepest descent line search					
set $\gamma_k = 1$					
while ( .not. Wolfe ) do					
update $\gamma_k = \gamma_k \rho$					
Wolfe $\Pi_p^{\nabla n}(\Delta \hat{\mathbf{u}}_{k-1} + \gamma_k \ \delta \Delta \hat{\mathbf{u}}_k) < \Pi_p^{\nabla n}(\Delta \hat{\mathbf{u}}_{k-1}) + c_1 \ \gamma_k \ \delta \Delta \hat{\mathbf{u}}_k^{\mathrm{T}} \mathbf{R}_{\mathrm{u}}(\Delta \hat{\mathbf{u}}_{k-1})$					
end					

The backtracking or steepest descent line search algorithm is shown in Algorithm 3. The idea is that the step length  $\gamma_k$  is reduced by a constant parameter  $\rho \in [1/10, 1/2]$ . Furthermore, a minimum value  $\gamma_{k,min}$ should not be reached as suggested in [50]. An important remark must be done on the Dirichelet boundary condition of the displacement field. The minimization outlined in (B.4) must hold for all the active degrees of freedom, i.e., the degrees of freedom that contribute to the minimization of the total energy in the time step. Therefore, the constrained degrees of freedom must be excluded from the algorithm. Yet, in order to avoid a too large difference in the increment update of the active degrees of freedom and the constrained degrees of freedom a not too small threshold must be used for the step length. The choosen value is  $\gamma_{k,min} = 1/2$ .

# 609 Appendix C. Linear activation criterions

The use of von-Mises plasticity with linear isotropic hardening results in the yield vector  $\mathbf{f}_{Y,e}$  to be a linear function of the plastic multiplier increment  $\Delta \hat{\lambda}_e$  as follows:

$$\mathbf{f}_{\mathbf{Y},e} = \int_{\Omega_{e}} \left[ \mathbf{N}_{\lambda}^{\mathrm{T}} \left( \sigma_{eq}^{tr} - 3G \,\Delta \lambda - \bar{\sigma}_{y0} - H \,\lambda \right) - c_{p} \,\mathbf{B}_{\lambda}^{\mathrm{T}} \,\nabla \lambda \right] \mathrm{d}\Omega_{e} = \\ = \int_{\Omega_{e}} \left[ \mathbf{N}_{\lambda}^{\mathrm{T}} \left( \sigma_{eq}^{tr} - \bar{\sigma}_{y0} - H \,\lambda_{n} \right) - c_{p} \,\mathbf{B}_{\lambda}^{\mathrm{T}} \,\nabla \lambda_{n} \right] \mathrm{d}\Omega_{e} + \\ \frac{\mathbf{f}_{Y,e}^{tr}}{\mathbf{f}_{Y,e}^{tr}} \tag{C.1}$$
$$- \left\{ \int_{\Omega_{e}} \left[ \left( 3G + H \right) \mathbf{N}_{\lambda}^{\mathrm{T}} \,\mathbf{N}_{\lambda} + c_{p} \,\mathbf{B}_{\lambda}^{\mathrm{T}} \,\mathbf{B}_{\lambda} \right] \mathrm{d}\Omega_{e} \right\} \Delta \hat{\lambda}_{e} \\ \frac{\mathbf{K}_{\lambda\lambda,e}}{\mathbf{K}_{\lambda\lambda,e}}$$

where the constant matrix  $\mathbf{K}_{\lambda\lambda,e}$  has already been defined in (A.3c), while the element trial yield vector is defined as:

$$\mathbf{f}_{\mathbf{Y},e}^{tr} := \int_{\Omega_e} \left[ \mathbf{N}_{\lambda}^{\mathrm{T}} \left( \sigma_{eq}^{tr} - \bar{\sigma}_{y0} - H \lambda_n \right) - c_p \, \mathbf{B}_{\lambda}^{\mathrm{T}} \, \mathbf{\nabla} \lambda_n \right] \mathrm{d}\Omega_e \tag{C.2}$$

<sup>614</sup> On the other hand, the choices of a quadratic degradation function and the use of an AT1 dissipation <sup>615</sup> functional for the phase field lead to the following definition of the phase-field activation vector  $\mathbf{f}_{D,e}$ :

$$\begin{split} \mathbf{f}_{\mathrm{D},e} &= \int_{\Omega_{e}} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \left[ 2(1-d) \, \tilde{\psi}_{0} - (f+1) \, \frac{3G_{c}}{8l_{0d}} + w_{\epsilon}' - \frac{\eta_{f}}{\Delta t} \, \Delta d \, \right] - \frac{3G_{c}l_{0d}}{4} \, \mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \, \nabla d \right\} \mathrm{d}\Omega_{e} = \\ &= \int_{\Omega_{e}} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \left[ 2(1-d_{n}) \, \tilde{\psi}_{0} - (f+1) \, \frac{3G_{c}}{8l_{0d}} + w_{\epsilon}' \right] - \frac{3G_{c}l_{0d}}{4} \, \mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \, \nabla d_{n} \right\} \mathrm{d}\Omega_{e} - \\ & \int_{\Omega_{e}} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \, \mathbf{N}_{\mathrm{d}} \left[ 2 \, \tilde{\psi}_{0} + \frac{\eta_{f}}{\Delta t} \right] + \frac{3G_{c}l_{0d}}{4} \, \mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \, \mathbf{B}_{\mathrm{d}} \right\} \mathrm{d}\Omega_{e} \right\} \\ & - \left\{ \int_{\Omega_{e}} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \, \mathbf{N}_{\mathrm{d}} \left[ 2 \, \tilde{\psi}_{0} + \frac{\eta_{f}}{\Delta t} \right] + \frac{3G_{c}l_{0d}}{4} \, \mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \, \mathbf{B}_{\mathrm{d}} \right\} \mathrm{d}\Omega_{e} \right\} \, \Delta \hat{\mathbf{d}}_{e} \end{split}$$

where the trial elastoplastic activation vector  $\mathbf{f}_{\mathrm{D},e}^{tr}$  and the matrix  $\mathbf{K}_{dd,e}$  have been defined:

$$\mathbf{f}_{\mathrm{D},e}^{tr} := \int_{\Omega_e} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \left[ 2(1-d_n) \,\tilde{\psi}_0 - (f+1) \,\frac{3G_c}{8l_{0d}} + w'_{\epsilon} \right] - \frac{3G_c l_{0d}}{4} \,\mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \,\mathbf{\nabla} d_n \right\} \mathrm{d}\Omega_e \tag{C.3a}$$

$$\mathbf{K}_{dd,e} := -\int_{\Omega_e} \left\{ \mathbf{N}_{\mathrm{d}}^{\mathrm{T}} \, \mathbf{N}_{\mathrm{d}} \left[ 2 \, \tilde{\psi}_0 + \frac{\eta_f}{\Delta t} \right] + \frac{3G_c l_{0d}}{4} \, \mathbf{B}_{\mathrm{d}}^{\mathrm{T}} \, \mathbf{B}_{\mathrm{d}} \right\} \mathrm{d}\Omega_e \tag{C.3b}$$

<sup>617</sup> Finally, the yielding and fracture activation criterions (53b) and (53c) can be written as follows:

$$\Delta \hat{\lambda} \ge \mathbf{0} \quad , \quad (\mathbf{f}_{Y}^{tr} + \mathbf{K}_{\lambda\lambda} \,\Delta \hat{\lambda}) \le \mathbf{0} \quad , \quad \Delta \hat{\lambda}^{\mathrm{T}} \left( \mathbf{f}_{Y}^{tr} + \mathbf{K}_{\lambda\lambda} \,\Delta \hat{\lambda} \right) = 0 \tag{C.4a}$$

$$\Delta \hat{\mathbf{d}} \ge \mathbf{0} \quad , \quad (\mathbf{f}_{\mathrm{D}}^{tr} + \mathbf{K}_{dd} \,\Delta \hat{\mathbf{d}}) \le \mathbf{0} \quad , \quad \Delta \hat{\mathbf{d}}^{\mathrm{T}} \left(\mathbf{f}_{\mathrm{D}}^{tr} + \mathbf{K}_{dd} \,\Delta \hat{\mathbf{d}}\right) = 0 \tag{C.4b}$$

They correspond to the Karush-Kuhn-Tucker conditions associated to the constrained minimization of the total energy with respect to the plastic multiplier and the phase field. The specific choices adopted for the constitutive functionals make them two symmetric linear complementarity problems of the standard form:

$$\mathbf{x} \ge \mathbf{0} \quad , \quad (\mathbf{q} + \mathbf{Q} \cdot \mathbf{x}) \le \mathbf{0} \quad , \quad \mathbf{x}^{\mathrm{T}} \left( \mathbf{q} + \mathbf{Q} \cdot \mathbf{x} \right) = \mathbf{0}$$

The solution of these variational inequalities is sought by means of a Projected Successive Over-Relaxation algorithm (PSOR) as introduced in [33]. It has been used for gradient plasticity [32] and in phase-field brittle fracture [34].

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