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Phase-field model for 2D cohesive-frictional shear fracture: An energetic formulation

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Abstract

This paper presents a phase-field model for cohesive-frictional shear fracture. The model is derived based on two energetic principles: the energy conservation law and a variational inequality of virtual work that serves as a stability condition. We show that all the governing equations for frictional fracture can be obtained from the above two principles, including the equilibrium condition, the phase-field evolution law and, most importantly, the yield function and flow rule for the plasticity-like frictional slip. The information of crack direction is naturally included in the flow rule. Theoretical and numerical results show that the proposed model is faithfully consistent with the Mohr-Coulomb theory of frictional failure in terms of the crack nucleation stress and direction. In addition, the presented phase-field model has an explicit frictional cohesive law.

Keywords: phase-field model, cohesive zone model, friction, shear fracture, crack angle, Mohr-Coulomb criterion, variational formulation, non-associative plasticity

1. Introduction

Fracture of solids is important in both theory and engineering applications, but is difficult to analyze and simulate especially when the crack path is unknown in advance. Physically, crack surfaces should be understood as a set of (traction-free or cohesive) internal boundaries of solid (Barenblatt, 1962). The displacement field may be discontinuous across the crack surface. In order to complete the theory, additional criteria and equations should be introduced to describe the nucleation and evolution of crack set (Erdogan and Sih, 1963; Bouchbinder, 2009). The resulting problem is much more difficult than the boundary value problems for partial differential equations we usually encounter, especially in the real 3D world with heterogeneities (Lebihain et al., 2022; Roch et al., 2023; He et al., 2023, 2024). This is because in the fracture problem, the spatial location of the boundary is itself the unknown to be solved.

To deal with the above problem, various theoretical and computational methods have been developed over the past three decades, including the damage mechanics (Peerlings et al., 1996; Frémond and Nedjar, 1996; Li and Ren, 2009; Xue et al., 2023), the cohesive element method (Xu and Needleman, 1994; Fan and Tadmor, 2019), peridynamics (Silling, 2000), extended finite element method (Moës et al., 1999), phase-field method (Francfort and Marigo, 1998; Bourdin et al., 2000; Karma et al., 2001; Freddi and Royer-Carfigani, 2010), and the recently proposed nonlocal macro-meso-scale consistent damage (NMMD) model (Lu and Chen, 2020; Chen et al., 2021; Ren et al., 2023, 2024b). Among them, the

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phase field fracture method is one of the theories with the closest connection to the traditional fracture mechanics and the most satisfactory numerical performance.

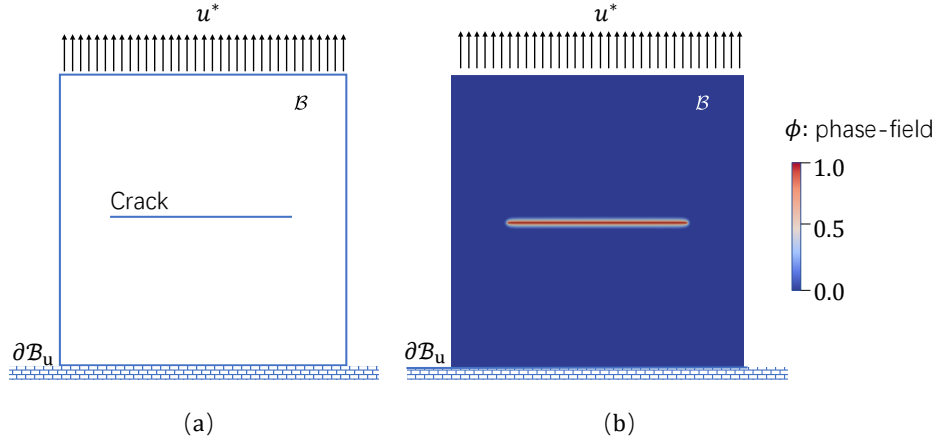


Figure 1: (a) The crack described as a sharp internal boundary and (b) the diffusive crack in the phase-field theory: The width of phase-field crack is probational to a length-scale parameter ℓ that appears in the total energy functional.

In the phase-field theory of fracture, an auxiliary continuous field variable ϕ , called phase-field, is introduced to mark the position of cracks. As shown in Fig. 1, the region where $0 < \phi < 1$ is interpreted as a phase-field crack, while the region where $\phi = 0$ represents the intact part of the solid. The width of a phase-field crack is controlled by a regularization length-scale parameter ℓ . The sharp crack pattern in fracture mechanics can be obtained as ℓ goes to zero. In the phase field theory of quasi-static fracture, complex crack evolution phenomena, including nucleation, propagation and merging, are interpreted in a unified way as the result of energy minimization. The expression of the total energy is assumed to be a functional of displacement field and phase-field. Once the expression for energy functional is given, the crack path can be obtained by finding the appropriate phase-field distribution that minimizes the total energy or, equivalently, solving the corresponding Euler-Lagrange equations. This continuous field description of crack avoids the difficulty of evolving free internal boundaries.

The phase-field approach is extremely extendable. By modifying the expression of energy functional and introducing more physical fields, the theory can be applied to a variety of engineering problems, such as thermal cracking (Ghasabeh and Göktepe, 2023; Zhou et al., 2024), corrosion cracking (Freddi and Mingazzi, 2022; Cui et al., 2021, 2022), fracture in quasi-crystals (Li et al., 2023), ductile fracture (Freddi and Royer-Carfagni, 2014; Han et al., 2022; Wang et al., 2023) and, cohesive fracture (Freddi and Iurlano, 2017; Feng and Wu, 2018; Feng et al., 2021; Bian et al., 2024). By introducing inertial and viscous effects into the governing equations, phase-field theory can be used to model complex behaviors in dynamic fracture such as crack branching (Karma and Lobkovsky, 2004; Hai and Li, 2021; Hai et al., 2024). By introducing the random field of material properties or by explicitly modeling the different phases at meso-scale, the stochastic failure and reliability of inhomogeneous materials such as concrete and composites also can be studied using the phase-field method (Hai and Li, 2022; Meshi et al., 2023; Vodička, 2023; Hai and Lyu, 2023).

However, there is no such thing as a free lunch. Due to the diffuse crack description used in the phase-field theory, the definition of crack direction becomes ambiguous, especially for a complex curved crack. This limits the application of phase-field fracture theory to many engineering problems. For example, in the modeling of mixed-mode cohesive fracture, hydraulic fracture, frictional contact, and Mohr-Coulomb-type failure, some key variables, such as the normal pressure, crack opening, and slip, cannot be defined when the crack surface normal is not well defined.

To address the above problem in a manner consistent with the diffusive crack description, one may introduce a new internal variable θ to characterize the direction of the potential crack at each material point. Steinke and Kaliske (2019) proposed an anisotropic stress decomposition method in a local coordinate system built on the potential crack surface. A similar local coordinate system was used by Fei and Choo (2020) to develop the phase-field method for frictional-shear fracture, and by Fei and Choo (2021) and Feng and Li (2022a) for mixed-mode fracture. The introduction of θ makes it possible to define the normal and shear stresses on a crack surface. It also allows us to distinguish between open and closed states of a phase-field crack. Clearly, how to determine the crack angle field θ is of vital importance. A common strategy is to intuitively force the crack angle θ to be 0, $\pi/4$ or $\pi/4 - \varphi/2$ based on the maximum tensile stress criterion, the maximum shear stress criterion or the Mohr-Coulomb criterion, where θ is the angle between the crack normal and the first principle direction of stress, and φ is the friction angle. However, this strategy is not always feasible for the phase-field fracture theory. In fact, upon a careful examination of the numerical results in the literature, it is not difficult to find that the actual crack angle predicted by the phase-field model may be very different from what we envisioned. For example, the compressive strength of materials such as rock is much higher than the tensile strength, which can be modelled by the friction effect in the Mohr-Coulomb criterion. We may introduce the friction effect by directly modifying the phase field driving force, which results in a hybrid (variationally inconsistent) phase-field model that can correctly predict the material's strength. However, as reported in the works of Zhou et al. (2019) and Haghghat and Santillán (2023), the obtained shear crack angle is roughly $\pi/4$ which is different from the theoretical value, $\pi/4 - \varphi/2$.

Feng and Li (2023b) found that the variational consistency may play a crucial role in accurately predicting crack angles in the phase-field theory. Feng and Li (2023b) proposed to write the total energy as a functional of displacement, phase-field, and the additional crack angle field, and the crack angle should be determined by rigorous energy minimization. The work of Feng and Li (2023b) results in a directional energy decomposition method, which proves to be perfectly suitable for mixed-mode cohesive fracture. However, the above energy minimization approach is not available for dissipative problems, for example, the cohesive-frictional fracture. As a fundamental theoretical question in the phase-field fracture method, how to correctly describe and predict the crack angle is still a challenging open issue. This question is also related to other fundamental problems, such as the crack nucleation criterion and strength theory.

In this paper, we put our efforts into developing the phase-field model for cohesive-frictional shear fracture, where the crack direction plays a crucial role. The model is derived based on an energetic formulation for rate-independent systems (Mielke and Roubíček, 2015). It has two energetic principles. One is the principle of energy conservation, and the other is the principle of inequality of virtual work that serves as a stability condition (Feng and Li, 2022a). This energetic formulation has succeeded in developing variational phase-field models for cohesive fracture (Pham et al., 2011; Pham and Marigo, 2013; Feng and Li, 2022a) and non-associative plastic fracture (Ulloa et al., 2021, 2022). In this paper, we show that all the governing equations for cohesive-frictional fracture can be obtained based on the aforementioned two energetic principles, including the equilibrium condition, the phase-field evolution law, and most importantly the yield function and flow rule for the plasticity-like frictional slip. It is noteworthy that the information about crack angle is naturally included in the flow rule.

This paper is organized as follows: Section 2 presents the general energetic formulation for the dissipative system. In Section 3, the phase-field model for cohesive-frictional fracture is derived based on the energetic formulation. Section 4 illustrates the numerical treatment of the proposed formulation that is implemented to perform some representative numerical examples of Section 5 that demonstrate the model's performance, including a direct shear test, a biaxial compression test, and a slope stability problem.

2. Energetic formulation for dissipative system

Let us consider a rate-independent system with all its displacement-like physical coordinates collected in $\mathbf{X} = \{X_1, X_2, \dots\}$. The potential energy of the system, denoted by $\mathcal{E}$, should be a function of $\mathbf{X}$ and possibly parameterized by a set of specified external loads $\mathbf{f}_{\text{ext}}$,

$$\mathcal{E}(\mathbf{X}) = \mathcal{E}_{\text{int}}(\mathbf{X}) - \mathbf{f}_{\text{ext}} \cdot \mathbf{X}. \quad (1)$$

We assume that the system is dissipative. That is, with an infinitesimal state increment $d\mathbf{X}$, there exists a non-negative energy dissipation

$$d\mathcal{D} = \mathbf{f}_{\text{diss}}(\mathbf{X}, \mathbf{N}_{d\mathbf{X}}) \cdot d\mathbf{X} \geq 0, \quad (2)$$

where $\mathbf{N}_{d\mathbf{X}}$ is the direction of $d\mathbf{X}$.

In general, the dissipation force $\mathbf{f}_{\text{diss}}$ not only depends on $\mathbf{X}$ but also on the direction of $d\mathbf{X}$, which makes the energy dissipation loading-path-dependent. Therefore, the dissipated energy up to the current time t can only be written as a time-accumulation of $d\mathcal{D}$ but not an increment of some potential energy. This fact is also highlighted in Eq. (2) by using the inexact differential symbol “ d ” that is commonly adopted in thermodynamics textbooks (Zemansky and Dittman, 1997; Kardar, 2007).

A rate-independent dissipative system can be analyzed based on two energetic conditions:

- The energy conservation law:

$$d\mathcal{E} + d\mathcal{D} = 0, \quad \text{or} \quad d\mathcal{E}_{\text{int}} + d\mathcal{D} = dW_{\text{ext}}, \quad (E)$$

where dW is the external work defined by $dW_{\text{ext}} = \mathbf{f}_{\text{ext}} \cdot d\mathbf{X}$.

- The first order stability condition: $\exists \bar{h} > 0 : \forall h \in [0, \bar{h}]$,

$$\delta\mathcal{E} + \delta\mathcal{D} \geq 0 \quad \forall \delta\mathbf{X} \text{ s.t. } \mathbf{X} + h\delta\mathbf{X} \in S_{\mathbf{X}}, \quad (S)$$

where $\delta\mathcal{E}$ denotes the first-order variation of the total potential energy,

$$\delta\mathcal{E} := \lim_{h \rightarrow 0^+} \frac{1}{h} \left[\mathcal{E}(\mathbf{X} + h\hat{\mathbf{X}}) - \mathcal{E}(\mathbf{X}) \right] = \frac{\partial\mathcal{E}}{\partial\mathbf{X}} \cdot \hat{\mathbf{X}} = \frac{\partial\mathcal{E}}{\partial\mathbf{X}} \cdot \delta\mathbf{X}, \quad (3)$$

$\delta\mathcal{D}$ is an inexact variation representing the virtual dissipation associated with the virtual displacement $\delta\mathbf{X}$,

$$\delta\mathcal{D} = \mathbf{f}_{\text{diss}}(\mathbf{X}, \mathbf{N}_{\delta\mathbf{X}}) \cdot \delta\mathbf{X}, \quad (4)$$

and $S_{\mathbf{X}}$ is the feasible region of $\mathbf{X}$ that takes into account all physical constraints such as boundary conditions and irreversibility.

Please note that, in condition (E) a real physical process during a time increment is concerned. For example, $d\mathcal{E}$ is the increment of potential energy associated with a real physical process $d\mathbf{X}$ during a time increment dt . Whereas in condition (S), the time is fixed at t and the terms $\delta\mathcal{E}$ and $\delta\mathcal{D}$ are the virtual works associated with an imaginary displacement $\delta\mathbf{X}$.

The physical meaning of condition (S) is as follows:

For the system to be stable at a state, it is necessary that the potential energy released by the system on any one of the feasible infinitesimal virtual paths is not greater than the energy to be dissipated.

The above physical meaning may be clearer if the inequality in condition (S) is rewritten as $-\delta\mathcal{E} \leq \delta\mathcal{D}$. The condition (S) is termed as the *principle of inequality of virtual works* (Feng and Li, 2022a, 2023a).

In general, all the governing equations of a quasi-static dissipative system can be derived from a combination of (E) and (S). This paradigm will be used in the following sections to construct our phase-field model of cohesive-frictional fracture.

3. Phase-field model of cohesive-frictional fracture

3.1. Regularization of displacement jump: crack strain

In a phase-field approach to cohesive fracture, the total strain can be split into two parts,

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^c, \quad (5)$$

where $\boldsymbol{\varepsilon}^e$ is the elastic strain and $\boldsymbol{\varepsilon}^c$ is the crack strain, used to regularize the crack surface displacement jump (Feng and Li, 2023b).

In general, the crack strain $\boldsymbol{\varepsilon}^c$ has two parts corresponding to the mode-I (tensile) and mode-II (shear) components of the crack surface displacement jump. Please refer to the work of Feng and Li (2023b) for a detailed discussion of this general mixed-mode cohesive fracture problem. In this paper, we only consider the shear fracture problem.

To be precise, we assume a traceless kinematic variable such that

$$\text{tr}(\boldsymbol{\varepsilon}^c) = 0. \quad (6)$$

This shear crack strain can be explicitly represented in a local coordinate system built on a crack surface (Fei and Choo, 2020; Feng and Li, 2022a, 2023b),

$$\boldsymbol{\varepsilon}^c = \frac{\gamma_n^c}{2} (\mathbf{n} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{n}), \quad (7)$$

where $\mathbf{n}$ is the crack normal and $\mathbf{m}$ is the unit vector perpendicular to $\mathbf{n}$.

As depicted in Fig.2, with the concept of crack strain, the crack surface slip can be regularized as the following spatial integration

$$\delta_s = \int_L \boldsymbol{\varepsilon}^c : (\mathbf{n} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{n}) dL = \int_L \gamma_n^c dL, \quad (8)$$

where L is a line running perpendicularly through the crack.

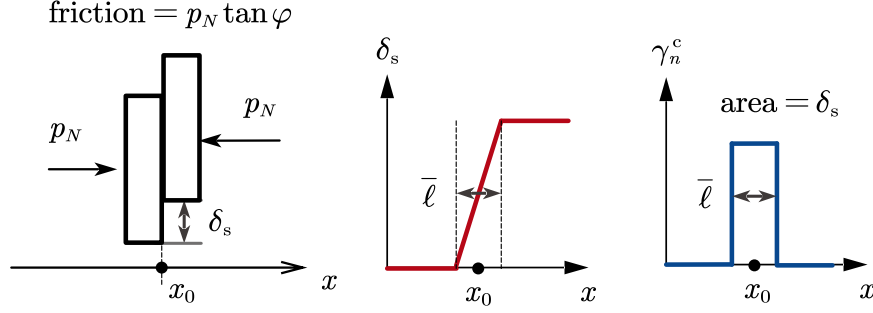


Figure 2: Schematic diagram of the regularization of crack slip in Eq. (8): φ is the friction angle. The width of diffusive phase-field cracks $\bar{\ell}$ is proportional to the length scale parameter ℓ in the phase-field models. The ratio depends on the model detail. For example, when linear cohesive law is used, $\bar{\ell} \approx 10\ell$ in our model.

3.2. Stored energy functional

In a variational phase-field model of fracture, the total stored energy density ψ can be written as the sum of the crack surface energy density ψ_{crack} and strain energy density ψ_{strain} ,

$$\psi = \psi_{\text{crack}} + \psi_{\text{strain}}. \quad (9)$$

The total potential energy of the solid $\mathcal{E}$ is a sum of the integration of ψ and the boundary term,

$$\mathcal{E} = \int_{\mathcal{B}} \psi \, dV - \int_{\partial\mathcal{B}_\sigma} \mathbf{t} \cdot \mathbf{u} \, dS, \quad (10)$$

where $\mathcal{B}$ is the space occupied by the solid, $\partial\mathcal{B}_\sigma$ is part of the boundary with specified traction loading $\mathbf{t}$, and $\mathbf{u}$ denotes the displacement.

According to the theory of Feng et al. (2021), the crack surface energy density for cohesive fracture problem has the following expression,

$$\psi_{\text{crack}} = \frac{G_c}{\ell} \left[(1 - \phi)^2 \omega(\phi) + \ell^2 |\nabla \phi|^2 \right], \quad (11)$$

where, as usual, ℓ is the length scale parameter that controls the width of the phase-field regularized crack, and G_c is the fracture energy.

The key function $\omega(\cdot)$ in Eq. (11), termed as the **intrinsic function of energy density**, can be determined by the material's cohesive law through a rigorous integral transform (Feng et al., 2021; Feng and Li, 2022b,a, 2023b),

$$\omega(\phi) = \frac{1}{\pi^2} \left(\frac{d}{d\phi} \int_0^\phi \frac{\Omega(\phi^*)}{\sqrt{(1 - \phi^*)^2 - (1 - \phi)^2}} d\phi^* \right)^2, \quad (12)$$

where $\Omega(\cdot)$ is the **intrinsic function of cohesive law** containing the information of material's cohesive law.

For example, if the material has a cohesive law of linearly decreasing form of Camacho and Ortiz (1996), then one has

$$\Omega_{\text{linear}}(\phi) = \phi \quad \text{and} \quad \omega_{\text{linear}}(\phi) = \frac{1}{\pi^2(1 - \phi)^2} (1 - (1 - \phi)^2). \quad (13)$$

Substituting Eq. (13) into Eq. (11) and performing a simple re-scaling of length parameter ℓ , the obtained expression for ψ_{crack} becomes the same as that in the model of Wu (2017),

$$\psi_{\text{crack}}^{\text{linear}} = \frac{G_c}{\pi \ell_0} \left[(2\phi - \phi^2) + \ell_0^2 |\nabla \phi|^2 \right], \quad \ell_0 = \pi \ell. \quad (14)$$

Alternative expressions of $\omega(\cdot)$ and $\Omega(\cdot)$ for other cohesive laws can be found in the original work of Feng et al. (2021) or Appendix A. We highlight that the integral transform Eq. (12) applies to any complex form of cohesive law.

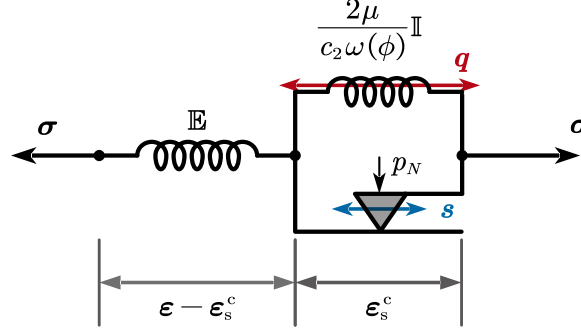


Figure 3: An illustration of the model’s strain energy ψ_{strain} , relative stress $\mathbf{s}$ and back stress $\boldsymbol{\epsilon}_s^c$: The strain energy is the sum of the energy stored in the two springs; $\mathbb{E}$ is the fourth-order elasticity tensor; $\mathbb{I}$ is the fourth-order identity tensor; The spring on the right is called the “crack spring”.

For the frictional shear problem, we propose the following expression for the strain energy density:

$$\psi_{\text{strain}}(\boldsymbol{\epsilon}, \phi, \boldsymbol{\epsilon}^c) = \frac{1}{2} (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^c) : \mathbb{E} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^c) + \frac{1}{2} \frac{2\mu}{c_2 \omega(\phi)} \|\boldsymbol{\epsilon}^c\|^2, \quad c_2 = \frac{G_c}{\ell} \left(\frac{\tau_{\text{cr}}^2}{2\mu} \right)^{-1}, \quad (15)$$

which can be understood intuitively through the system of springs illustrated in Fig. 3. Here, $\mathbb{E}$ is the fourth-order elasticity tensor and τ_{cr} is the material’s inherent shear strength without consideration of friction effect. The material parameter τ_{cr} can also be interpreted as the nucleation stress of a shear crack or shear zone.

As illustrated in Fig. 3, by introducing the fourth-order identity tensor $\mathbb{I}$, the energy in the “crack spring” (second term of the expression of ψ_{strain} in Eq. (15)), may be rewritten as $\boldsymbol{\epsilon}^c : \mathbb{H} : \boldsymbol{\epsilon}^c / 2$ with $\mathbb{H} = 2\mu / (c_2 \omega(\phi)) \mathbb{I}$.

The function $\omega(\cdot)$ in Eq. (15) plays the role of a prefactor of the compliance for the “crack spring” (see Fig. 3). For an intact solid, the stiffness of the crack spring should be infinite so that the crack strain and the crack opening are zero. This requires that $\omega(0^+) = 0^+$. On the other hand, for a fully broken solid, the stiffness of the crack spring should be zero and the compliance should be infinity, i.e., $\omega(1) = \infty^+$. These properties were discussed in the work of Feng and Li (2023b).

As demonstrated in the work of Feng and Li (2023b), if there is no friction or any other dissipation mechanism, the cohesive fracture problem can be formulated as an energy minimization problem in the spirit of Francfort and Marigo (1998). In that case, the crack strain can be eliminated as a micro-variable through a homogenization process, which dramatically simplifies the expression of energy density. However, the approach in Feng and Li (2023b) does not apply for the frictional shear fracture problem of interest in this work. A description of frictional dissipation is required to complete our theory.

3.3. Frictional energy dissipation

In a variational phase-field fracture model, the surface energy, or the fracture energy, is assumed to be stored in the state function ψ_{crack} in Eq. (11). Therefore, this portion of energy can be considered conservative. The work done by friction, on the other hand, is generally dissipated through heat and is therefore considered the true and only dissipation mechanism in this article.

To describe frictional energy dissipation, the incremental theory in Eq. (2) should be adopted. We propose that in a phase-field regularized model of frictional shear fracture, the energy dissipation associated with an increment of shear crack strain $d\boldsymbol{\varepsilon}^c$ can be expressed as

$$d\mathcal{D} = \int_{\mathcal{B}} \mathbf{f}_N : d\boldsymbol{\varepsilon}^c dV, \quad (16)$$

where $\mathbf{f}_N$ is a friction-like force that depends on the stress state and the direction of $d\boldsymbol{\varepsilon}^c$.

Note that the crack may change its propagation direction. Thus the direction of $d\boldsymbol{\varepsilon}^c$ is not necessarily the same as the direction of $\boldsymbol{\varepsilon}^c$ in Eq. (7). In general, we have

$$d\boldsymbol{\varepsilon}^c = \frac{1}{2} d\gamma_\alpha^c (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \quad (17)$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are unit vectors perpendicular to each other; $\boldsymbol{\alpha}$ is not necessarily equal to $\mathbf{n}$ in Eq. (7).

Eq. (17) can be compactly rewritten as

$$d\boldsymbol{\varepsilon}^c = \|d\boldsymbol{\varepsilon}^c\| \mathbf{N}, \quad (18)$$

where

$$\|d\boldsymbol{\varepsilon}^c\| = \sqrt{d\boldsymbol{\varepsilon}^c : d\boldsymbol{\varepsilon}^c} = \frac{\sqrt{2}}{2} |d\gamma_\alpha^c|, \quad (19)$$

$$\mathbf{N} = \frac{\sqrt{2}}{2} \text{sgn}(d\gamma_\alpha^c) (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \quad \|\mathbf{N}\| = 1. \quad (20)$$

Note that we have constrained ourselves in a 2D setting.

The friction stress $\mathbf{f}_N$ in Eq. (16) is selected to be of the Coulomb's type,

$$\mathbf{f}_N = \text{sgn}(d\gamma_\alpha^c) p_N \tan \varphi (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \quad (21)$$

or

$$\mathbf{f}_N = \|\mathbf{f}_N\| \mathbf{N}, \quad \|\mathbf{f}_N\| = \sqrt{2} p_N \tan \varphi, \quad (22)$$

where the subscript “N” indicates that the friction $\mathbf{f}_N$ depends on the direction of the shear crack strain increment, and φ is the material's friction angle.

The normal pressure $p_N \geq 0$ is defined by

$$p_N = \min\{p_\alpha, p_\beta\}, \quad p_\alpha = \langle -\boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \rangle, \quad p_\beta = \langle -\boldsymbol{\sigma} : (\boldsymbol{\beta} \otimes \boldsymbol{\beta}) \rangle, \quad (23)$$

where $\langle \square \rangle = (|\square| + \square)/2$ are the Macaulay brackets that take the positive value, and $\boldsymbol{\sigma}$ is the stress tensor in the usual sense, $\boldsymbol{\sigma} = \mathbb{E} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^c)$.

In Eq. (23), the choice of a smaller normal pressure, and thus a smaller friction force, is made to take into account *the most dangerous situation* in shear slip. This choice is consistent with the principle of

virtual work inequality (S) and makes the friction $\mathbf{f}_N$ in Eq. (21) uniquely determined by $\mathbf{N}$ when the stress state is given.

It is easy to check that the dissipation introduced here is always non-negative. Substituting Eq. (18) and Eq. (22) into Eq. (16) gives

$$\mathrm{d}\mathcal{D} = \int_{\mathcal{B}} \mathbf{f}_N : \mathrm{d}\boldsymbol{\varepsilon}^c \, \mathrm{d}V = \int_{\mathcal{B}} \|\mathbf{f}_N\| \|\mathrm{d}\boldsymbol{\varepsilon}^c\| \, \mathrm{d}V = \int_{\mathcal{B}} p_N \tan \varphi |\mathrm{d}\gamma_\alpha^c| \mathrm{d}V \geq 0. \quad (24)$$

According to the local uniform stress assumption (see section 5 in Feng et al. (2021)), as $\ell \rightarrow 0$ the width of a phase-field crack goes to zero and the stress can be regarded as a constant across the crack. Therefore, for a sufficiently small ℓ , the energy dissipation in a small segment of phase-field crack of length Δa can be written as

$$\mathrm{d}\mathcal{D} = (p_N \tan \varphi \Delta a) \int_L |\mathrm{d}\gamma_\alpha^c| \mathrm{d}L = (p_N \tan \varphi \Delta a) |\mathrm{d}\delta_s|, \quad (25)$$

where the definition of the regularized crack surface slip δ_s in Eq. (8) is used to obtain the second equation.

Eq. (25) correctly recovers the energy dissipation in the sharp crack limit. That is, the dissipated energy is equal to the work done by the Coulomb-type friction force $p_N \tan \varphi \Delta a$ over the crack slip $|\mathrm{d}\delta_s|$.

3.4. Governing equations

With the expressions for potential energy and dissipation in hand (see Eq. (10) and Eq. (16)), now we can apply the principle of inequality of virtual work, aided by the energy conservation law, to obtain all the governing equations of our phase-field regularized frictional shear fracture problem. In what follows, we present this procedure in detail.

According to the principle of inequality of virtual work (S), for a state of the solid $\mathbf{X} = (\mathbf{u}, \boldsymbol{\varepsilon}^c, \phi)$ to be locally stable, one must have

$$\delta\mathcal{E} + \delta\mathcal{D} \geq 0, \quad (26)$$

for all the physically admissible $\delta\mathbf{X} = (\delta\mathbf{u}, \delta\boldsymbol{\varepsilon}^c, \delta\phi)$. To be precise, the constraints on the variations are as follows:

$$\delta\mathbf{u} = \mathbf{0} \quad \text{on } \partial\mathcal{B}_u; \quad (27a)$$

$$\mathrm{tr}(\delta\boldsymbol{\varepsilon}^c) = 0 \quad \text{in } \mathcal{B} \cup \partial\mathcal{B}; \quad (27b)$$

$$\text{There exists a positive } \bar{h} \text{ such that for all } h \in [0, \bar{h}], \quad \phi + h\delta\phi \geq \phi_{i-1} \text{ in } \mathcal{B} \cup \partial\mathcal{B}. \quad (27c)$$

The above conditions are respectively derived from the displacement boundary condition, the property of pure shear crack strain in Eq. (17), and the strong irreversibility condition $\phi \geq \phi_{i-1}$ where ϕ_{i-1} denotes the phase-field (damage) at the previous time step¹. Note that the inequality in (27c) cannot be replaced by “ $\phi + \delta\phi \geq \phi_{i-1}$ ”. Actually, $\delta\phi$ denotes the “direction” of a perturbation while h denotes the magnitude (See the definition in Eq. (3) or the work of Pham et al. (2011)). For a more detailed

¹Here a time discretization $\{t_i\}, i \in \mathbb{N}$, is tacitly assumed. When the time step goes to zero, a continuous problem can be obtained as a limit (Francfort and Larsen, 2003).

discussion of irreversibility in the phase-field fracture theory, please refer to the work of [Xue and Ren \(2024\)](#).

3.4.1. Equilibrium equation

Performing the first variation on Eq. (10), we have

$$\delta\mathcal{E} = \int_{\mathcal{B}} \left(\frac{\partial\psi}{\partial\phi} \delta\phi + \frac{\partial\psi}{\partial\nabla\phi} \cdot \nabla\delta\phi \right) dV + \int_{\mathcal{B}} \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} : \delta\boldsymbol{\varepsilon} dV + \int_{\mathcal{B}} \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^c} : \delta\boldsymbol{\varepsilon}^c dV - \int_{\partial\mathcal{B}_\sigma} \mathbf{t} \cdot \delta\mathbf{u} dS. \quad (28)$$

The virtual energy dissipation follows from Eq. (16) as

$$\delta\mathcal{D} = \int_{\mathcal{B}} \mathbf{f}_N : \delta\boldsymbol{\varepsilon}^c dV, \quad (29)$$

where the friction stress $\mathbf{f}_N$ now depends on the direction of the variation $\delta\boldsymbol{\varepsilon}^c$.

Substituting Eqs. (28) and (29) into Eq. (26), applying Cauchy's formula $\mathbf{t} = \bar{\mathbf{n}} \cdot \boldsymbol{\sigma}$, integral by parts and the divergence theorem, we have

$$\begin{aligned} \delta\mathcal{E} + \delta\mathcal{D} = & \int_{\mathcal{B}} \left(\frac{\partial\psi}{\partial\phi} - \nabla \cdot \frac{\partial\psi}{\partial\nabla\phi} \right) \delta\phi dV + \int_{\mathcal{B}} \left(-\nabla \cdot \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} \right) \cdot \delta\mathbf{u} dV + \int_{\mathcal{B}} \left(\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^c} + \mathbf{f}_N \right) : \delta\boldsymbol{\varepsilon}^c dV \\ & - \int_{\partial\mathcal{B}_\sigma} \bar{\mathbf{n}} \cdot \left(\boldsymbol{\sigma} - \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} \right) \cdot \delta\mathbf{u} dS + \int_{\partial\mathcal{B}} \bar{\mathbf{n}} \cdot \frac{\partial\psi}{\partial\nabla\phi} \delta\phi dS \geq 0, \end{aligned} \quad (30)$$

where $\bar{\mathbf{n}}$ is the normal of the boundary $\partial\mathcal{B}$.

First, let $\delta\phi = 0$, $\delta\boldsymbol{\varepsilon}^c = \mathbf{0}$ and $\delta\mathbf{u} \neq 0$. Due to the arbitrariness of $\delta\mathbf{u}$ in $\mathcal{B}$ and on $\partial\mathcal{B}_\sigma$, it follows from Eq. (30) that

$$\boldsymbol{\sigma} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} = \mathbb{E} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^c) \quad (31)$$

and

$$-\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \quad (32)$$

which are the stress-strain constitutive relation and the equilibrium equation, respectively.

Eq. (32) serves as the governing equation for the displacement field.

3.4.2. Evolution equations for phase-field

Let $\delta\boldsymbol{\varepsilon}^c = \mathbf{0}$ and $\delta\phi \neq 0$. Substituting Eqs. (31) and (32) into Eq. (30), we have

$$\int_{\mathcal{B}} \frac{\delta\mathcal{E}}{\delta\phi} \delta\phi dV + \int_{\partial\mathcal{B}} \bar{\mathbf{n}} \cdot \frac{\partial\psi}{\partial\nabla\phi} \delta\phi dS \geq 0, \quad (33)$$

where

$$\frac{\delta\mathcal{E}}{\delta\phi} = \frac{\partial\psi}{\partial\phi} - \nabla \cdot \frac{\partial\psi}{\partial\nabla\phi} \quad (34)$$

is the functional derivative of total energy $\mathcal{E}$ with respect to ϕ .

Inequality (33) should hold for all $\delta\phi$ that do not violate the constraint in Eq. (27c), $\exists h > 0 : \phi + h\delta\phi \geq \phi_{i-1}$. This is a variational inequality problem with an inequality constraint (irreversibility).

Its solution can be obtained from the standard Kuhn-Tucker conditions (see [Appendix B](#) for the proof):

$$\frac{\delta \mathcal{E}}{\delta \phi} \dot{\phi} = 0, \quad \frac{\delta \mathcal{E}}{\delta \phi} \geq 0 \quad \text{and} \quad \dot{\phi} \geq 0 \quad \text{in } \mathcal{B}, \quad (35)$$

and

$$\left(\bar{\mathbf{n}} \cdot \frac{\partial \psi}{\partial \nabla \phi} \right) \dot{\phi} = 0, \quad \bar{\mathbf{n}} \cdot \frac{\partial \psi}{\partial \nabla \phi} \geq 0 \quad \text{and} \quad \dot{\phi} \geq 0 \quad \text{on } \partial \mathcal{B}, \quad (36)$$

where $\dot{\phi} = d\phi/dt \propto (\phi_i - \phi_{i-1})$ is the derivative with respect to time or pseudo-time.

Eq. (35) collects the governing inequalities for the phase-field evolution.

Using the specific expressions for energy densities in Eqs. (9), (11) and (15), the expression for $\delta \mathcal{E}/\delta \phi$ of our model is as follows:

$$\frac{\delta \mathcal{E}}{\delta \phi} = \mathcal{F}_{\text{resistive}} - \mathcal{F}_{\text{driving}}, \quad (37)$$

where

$$\mathcal{F}_{\text{resistive}} = G_c \left[\frac{\partial \varphi_{\text{crack}}}{\partial \phi} - \nabla \cdot \frac{\partial \varphi_{\text{crack}}}{\partial \nabla \phi} \right] = \frac{G_c}{\ell} \left[\frac{d}{d\phi} [(1 - \phi)^2 \omega(\phi)] - 2\ell^2 \nabla^2 \phi \right], \quad (38)$$

$$\mathcal{F}_{\text{driving}} = -\frac{\partial \varphi_{\text{strain}}}{\partial \phi} = -c_2 \omega'(\phi) \frac{1}{2} \frac{\|\mathbf{q}\|^2}{2\mu}, \quad \mathbf{q} = \frac{2\mu}{c_2 \omega(\phi)} \boldsymbol{\varepsilon}^c. \quad (39)$$

Physically, $\mathcal{F}_{\text{resistive}}$ is the resistive force for phase-field evolution due to the increase of surface energy, $\mathcal{F}_{\text{driving}}$ is the driving force due to the drop of strain energy, and $\mathbf{q}$ is the stress in the “crack spring” (see Fig. (3)). In the context of plastic mechanics, $\mathbf{q}$ is known as the back stress ([Simo and Hughes, 2006](#)).

Finally, we note that special care should be taken with the driving force $\mathcal{F}_{\text{driving}}$ when $\phi = 0$.

For an intact solid, both of the crack strain and the compliance of “crack spring” are zero. Namely, when $\phi = 0$, we have $\boldsymbol{\varepsilon}^c = \mathbf{0}$ and $\omega(0) = 0$. Therefore when $\phi = 0$, the back stress $\mathbf{q}$ cannot be calculated directly from Eq. (39) and thus the driving force $\mathcal{F}_{\text{driving}}$ is undetermined.

To derive the driving force at $\phi = 0$ requires some knowledge in Section 3.4.3. For the reader's convenience, we give the result directly here and leave the derivation in [Appendix C](#):

$$\mathcal{F}_{\text{driving}} = -c_2 \omega'(\phi) \frac{1}{2} \frac{\|\mathbf{q}\|^2}{2\mu} = g_2'(\phi) \frac{1}{2\mu} \langle |\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi \rangle^2 \quad \text{if } \phi = 0, \quad (40)$$

where

$$g_2(\phi) = \frac{1}{1 + c_2 \omega(\phi)} \quad (41)$$

is the energy degradation function in a cohesive fracture problem ([Feng et al., 2021](#); [Feng and Li, 2022a, 2023b](#)), $\bar{\sigma}_{\alpha\beta}$ is the nominal shear stress on the potential crack surface, $\bar{\sigma}_{\alpha\beta} = \bar{\boldsymbol{\sigma}} : (\boldsymbol{\alpha} \otimes \boldsymbol{\beta})$, $\bar{\boldsymbol{\sigma}} = \mathbb{E} : \boldsymbol{\varepsilon}$ is the nominal stress tensor, $\boldsymbol{\alpha}$ is the normal vector of the potential crack, p_N is the normal pressure defined in Eq. (23), and φ is the friction angle. The direction of $\boldsymbol{\alpha}$ will be discussed in detail in Section

3.4.3.

In numerical simulations, we adopt Eq. (40) if $\phi \leq 1 \times 10^{-20}$ and Eq. (39) otherwise.

The energy degradation function Eq. (41) is closely related to the intrinsic function $\omega(\cdot)$ which can be derived mathematically based on the integral transform Eq. (12). We note that in the newly proposed NMMD model, the energy degradation function can be physically quantified on the meso-scale (Chen et al., 2021; Ren et al., 2024b), which provides a different but interesting perspective from the phase-field model.

3.4.3. Evolution equations for crack strain

Let $\delta\phi = 0$ and $\delta\epsilon^c \neq \mathbf{0}$. Substituting Eqs. (31) and (32) into Eq. (30), and using the expression for ψ given by Eqs. (9), (11) and (15), we have

$$\int_{\mathcal{B}} (\mathbf{s} - \mathbf{f}_N) : \delta\epsilon^c dV \leq 0 \quad \forall \delta\epsilon^c \quad \text{s.t.} \quad \text{tr}(\delta\epsilon^c) = 0, \quad (42)$$

where $\mathbf{s}$ is the thermodynamic force conjugated to the crack strain ϵ^c ,

$$\mathbf{s} = -\frac{\partial\psi}{\partial\epsilon^c} = \boldsymbol{\sigma} - \mathbf{q}, \quad \text{and} \quad \mathbf{q} = \frac{2\mu}{c_2\omega(\phi)}\epsilon^c. \quad (43)$$

In the context of plastic mechanics (Simo and Hughes, 2006), $\mathbf{s}$ and $\mathbf{q}$ are known as the *relative stress* and *back stress*, respectively.

Similar to those in Eq. (18) and Eq. (22), we have

$$\delta\epsilon^c = \|\delta\epsilon^c\|\mathbf{N} \quad \text{and} \quad \mathbf{f}_N = \sqrt{2}p_N \tan\varphi \mathbf{N}, \quad (44)$$

where

$$\mathbf{N} = \frac{\sqrt{2}}{2} \text{sgn}(\delta\gamma_\alpha^c)(\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \quad \|\mathbf{N}\| = 1. \quad (45)$$

Substituting Eq. (44) into Eq. (42) and noticing the arbitrariness of $\mathcal{B}$, we arrive the following optimization problem:

$$\max_{\mathbf{N}} F(\mathbf{s}, \boldsymbol{\sigma}, \mathbf{N}) \leq 0 \quad \text{s.t.} \quad \|\mathbf{N}\| = 1, \quad (46)$$

where

$$F(\mathbf{s}, \boldsymbol{\sigma}, \mathbf{N}) = \frac{\sqrt{2}}{2} \mathbf{s} : \mathbf{N} - p_N \tan\varphi. \quad (47)$$

Please note that the normal pressure p_N also depends on $\mathbf{N}$, which makes the problem strongly nonlinear.

Eq. (46) plays the role of yield surface for our plasticity-like frictional shear problem.

To show that the maximizer $\mathbf{N}$ of the problem in Eq. (46) is indeed the real direction of shear crack strain increment, we need the aid of energy conservation law (E). During an infinitesimal time increment dt , we have

$$d\mathcal{E}_{\text{int}} + d\mathcal{D} = dW_{\text{ext}}, \quad (48)$$

where $\mathrm{d}W_{\text{ext}}$ is the external work,

$$\mathrm{d}W_{\text{ext}} = \int_{\partial\mathcal{B}_\sigma} \mathbf{t} \cdot \mathrm{d}\mathbf{u} \, \mathrm{d}S, \quad (49)$$

$\mathrm{d}\mathcal{E}_{\text{int}}$ is the increment of internal energy,

$$\mathrm{d}\mathcal{E}_{\text{int}} = \int_{\mathcal{B}} \mathrm{d}\psi \, \mathrm{d}V, \quad (50)$$

and $\mathrm{d}\mathcal{D}$ is the energy dissipated by friction,

$$\mathrm{d}\mathcal{D} = \int_{\mathcal{B}} \mathbf{f}_N : \mathrm{d}\boldsymbol{\varepsilon}^c \, \mathrm{d}V = \int_{\mathcal{B}} p_N \tan \varphi |\mathrm{d}\gamma_\alpha^c| \, \mathrm{d}V. \quad (51)$$

Substituting Eqs. (49), (50) and (51) into Eq. (48), performing integral by parts and divergence theorem, we have

$$\begin{aligned} \mathrm{d}\mathcal{E}_{\text{int}} + \mathrm{d}\mathcal{D} - \mathrm{d}W_{\text{ext}} = & \int_{\mathcal{B}} \frac{\partial \mathcal{E}}{\partial \phi} \mathrm{d}\phi \, \mathrm{d}V - \int_{\mathcal{B}} \left(\nabla \cdot \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} \right) \cdot \mathrm{d}\mathbf{u} \, \mathrm{d}V - \int_{\mathcal{B}} (\mathbf{s} - \mathbf{f}_N) : \mathrm{d}\boldsymbol{\varepsilon}^c \, \mathrm{d}V \\ & - \int_{\partial\mathcal{B}_\sigma} \bar{\mathbf{n}} \cdot \left(\boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} \right) \cdot \mathrm{d}\mathbf{u} \, \mathrm{d}S + \int_{\partial\mathcal{B}} \bar{\mathbf{n}} \cdot \frac{\partial \psi}{\partial \nabla \phi} \mathrm{d}\phi \, \mathrm{d}S = 0. \end{aligned} \quad (52)$$

Using the stress-strain relation Eq. (31), the linear momentum balance equation Eq. (32), and the complementary conditions in Eq. (35) and Eq. (36), one can simplify Eq. (52) as follows:

$$\int_{\mathcal{B}} (\mathbf{s} - \mathbf{f}_N) : \mathrm{d}\boldsymbol{\varepsilon}^c \, \mathrm{d}V = 0. \quad (53)$$

Substituting $\mathrm{d}\boldsymbol{\varepsilon}^c = \|\mathrm{d}\boldsymbol{\varepsilon}^c\| \mathbf{N}$ and $\mathbf{f}_N = \sqrt{2} p_N \tan \varphi \mathbf{N}$ (see Eq. (18) and Eq. (22)) into Eq. (53), and dividing the result by $\sqrt{2}$, we have

$$F(\mathbf{s}, \boldsymbol{\sigma}, \mathbf{N}) \|\mathrm{d}\boldsymbol{\varepsilon}^c\| = \left(\frac{\sqrt{2}}{2} \mathbf{s} : \mathbf{N} - p_N \tan \varphi \right) \|\mathrm{d}\boldsymbol{\varepsilon}^c\| = 0, \quad (54)$$

where $F(\mathbf{s}, \mathbf{N})$ is defined in Eq. (47) and now $\mathbf{N}$ is the actual incremental direction of crack strain:

$$\mathbf{N} = \frac{\sqrt{2}}{2} \text{sgn}(\mathrm{d}\gamma_\alpha) (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \quad \mathrm{d}\gamma_\alpha = \mathrm{d}\boldsymbol{\varepsilon}^c : (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}). \quad (55)$$

Note that the local stability condition requires $\max_{\mathbf{N}} F \leq 0$ (see Eq. (46)), but the energy conservation law requires $F = 0$ if $\mathrm{d}\boldsymbol{\varepsilon}^c \neq \mathbf{0}$ (see Eq. (54)). This indicates that when $\mathrm{d}\boldsymbol{\varepsilon}^c \neq \mathbf{0}$, the actual incremental direction of the crack strain *does* maximize the function F defined in Eq. (47). That is,

$$\mathbf{N} = \arg \max_{\|\mathbf{N}\|=1} \left(\frac{\sqrt{2}}{2} \mathbf{s} : \mathbf{N} - p_N \tan \varphi \right), \quad \text{if } \dot{\boldsymbol{\varepsilon}}^c \neq \mathbf{0}. \quad (56)$$

The above problem has a closed-form solution. Next, we sketch the solving procedure.

We first note that

$$\mathbf{s} : \mathbf{N} / \sqrt{2} = \text{sgn}(\text{d}\gamma_\alpha) s_{\alpha\beta} \leq |s_{\alpha\beta}|, \quad (57)$$

where

$$s_{\alpha\beta} = \mathbf{s} : (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}) / 2, \quad (58)$$

and the equality $\mathbf{s} : \mathbf{N} / \sqrt{2} = |s_{\alpha\beta}|$ holds when

$$\text{sgn}(\text{d}\gamma_\alpha) = \text{sgn}(s_{\alpha\beta}). \quad (59)$$

In addition, it follows from Eq. (23) that p_N depends on $\mathbf{N}$ only through $\boldsymbol{\alpha}$ or $\boldsymbol{\beta}$ but not the sign of $\text{d}\gamma_\alpha$. Therefore, we conclude that Eq. (59) is a condition that needs to be satisfied for the solution of the problem in Eq. (56).

Without loss of generality, we assume that $\boldsymbol{\alpha}$ denotes the normal of the crack surface. That is, p_α is assumed to be smaller than p_β in Eq. (23). Let us denote by θ the angle between $\boldsymbol{\alpha}$ and the direction of the first principal stress σ_1 . With these preparations, the incremental direction $\mathbf{N}$ of the crack strain is uniquely determined by θ .

Substituting the condition Eq. (59) into Eq. (56), we obtain

$$\theta = \arg \max_{-\pi/4 < \theta \leq \pi/4} (|s_{\alpha\beta}| - p_N \tan \varphi). \quad (60)$$

Since $\boldsymbol{\alpha}$ is taken as the crack normal, according to Eq. (23), we have $p_\alpha \leq p_\beta$ and hence $\sigma_{\alpha\alpha} \geq \sigma_{\beta\beta}$, which implies that $|\theta| \leq \pi/4$.

The physical meaning of Eq. (60) is clear and consistent with the Mohr-Coulomb theory. It means that the net driving force (shear stress minus friction) is maximized at the actual crack plane, as this is the most dangerous situation.

The problem in Eq. (60) has a closed-form solution as follows (see Appendix D for the derivation):

$$\theta = \begin{cases} \theta_1, & \sigma_{\alpha\alpha}(\theta_1) < 0, \\ \theta_2, & \sigma_{\alpha\alpha}(\theta_2) > 0, \\ \theta_3, & \text{otherwise,} \end{cases} \quad (61)$$

where $\sigma_{\alpha\alpha}(\theta) = \boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = a_\sigma + r_\sigma \cos(2\theta)$, $a_\sigma = (\sigma_1 + \sigma_2)/2$, $r_\sigma = (\sigma_1 - \sigma_2)/2$, σ_1 and σ_2 are the first two principal values of $\boldsymbol{\sigma}$,

$$\theta_1 = -\text{sgn}(\theta_{s_1}^{\text{eff}}) [\pi/4 - \arctan(A)/2], \quad (62a)$$

$$\theta_2 = -\text{sgn}(\theta_{s_1}^{\text{eff}}) \pi/4 + \theta_{s_1}^{\text{eff}}, \quad (62b)$$

$$\theta_3 = -\text{sgn}(\theta_{s_1}^{\text{eff}}) \arccos(-a_\sigma/r_\sigma)/2, \quad (62c)$$

and

$$\theta_{s_1}^{\text{eff}} = \begin{cases} \theta_{s_1}, & |\theta_{s_1}| \leq \pi/4, \\ \theta_{s_1} - \text{sgn}(\theta_{s_1})\pi/2, & \pi/4 < |\theta_{s_1}| \leq \pi/2, \end{cases} \quad (63)$$

with θ_{s_1} the angle between the first principal direction of $\mathbf{s}$ and the first principal direction of $\boldsymbol{\sigma}$.

In Eq. (62a), the auxiliary variable A is defined as follows:

$$A = \text{sgn}(\theta_{s_1}^{\text{eff}}) \tan(2\theta_{s_1}^{\text{eff}}) + \tan(\varphi) \sec(2\theta_{s_1}^{\text{eff}}) r_{\sigma}/r_s, \quad (64)$$

where φ is the friction angle and $r_s = (s_1 - s_2)/2$ with s_1 and s_2 the first two principal values of $\mathbf{s}$.

Due to the periodicity, it is sufficient to only consider the values of θ_{s_1} in an interval of length π . In Eq. (63) we have specified that $-\pi/2 < \theta_{s_1} \leq \pi/2$.

Now with the results in Eq. (59) and Eq. (61), the crack strain flow direction $\mathbf{N}$ in Eq. (55) can be determined from the stress state $\{\mathbf{s}, \boldsymbol{\sigma}\}$.

Letting $\boldsymbol{\varepsilon}^c = \mathbf{0}$, the crack nucleation angle in compression is obtained from Eq. (61) as $\pm(\pi/4 - \varphi/2)$, which is consistent with the Mohr-Coulomb theory. One can also prove that the crack angle will not change during a monotonic stress loading.

Finally, the governing equations for the evolution of $\boldsymbol{\varepsilon}^c$ can be summarized as a set of Kuhn–Tucker conditions,

$$F(\mathbf{s}, \boldsymbol{\sigma}, \mathbf{N})\dot{\lambda} = 0, \quad F(\mathbf{s}, \boldsymbol{\sigma}, \mathbf{N}) \leq 0 \quad \text{and} \quad \dot{\lambda} \geq 0, \quad (65)$$

and a flow rule,

$$\dot{\boldsymbol{\varepsilon}}^c = \dot{\lambda} \mathbf{N}, \quad \dot{\lambda} = \|\dot{\boldsymbol{\varepsilon}}^c\|, \quad (66)$$

where the yield function $F(\mathbf{s}, \boldsymbol{\sigma}, \mathbf{N})$ is defined in Eq. (47) and the flow direction $\mathbf{N}$ is determined by $\{\mathbf{s}, \boldsymbol{\sigma}\}$ through Eqs. (55), (59) and (61).

It is easy to see that the flow rule obtained here is non-associative. This supports the idea that non-associative flow rules can be obtained via variational formulation (Francfort, 2018; Ulloa et al., 2021).

3.5. Frictional cohesive law

The cohesive law of the presented model can be derived by using the same method in our previous works (Feng et al., 2021; Feng and Li, 2022a,b, 2023b). Here we skip the derivation process and give the result directly. Readers interested in the derivation are referred to our previous works.

The frictional cohesive law of the presented model can be expressed by a set of parametric equations:

$$\delta_s/\delta_{\text{ch},s} = \Omega(\phi^*) \quad \text{and} \quad (\tau_s - p_N \tan \varphi)/\tau_{\text{cr}} = 1 - \phi^*, \quad (67)$$

where ϕ^* is the parameter with a physical meaning of damage (Feng and Li, 2022b), $\delta_{\text{ch},s} = 2G_c/\tau_{\text{cr}}$ is a characteristic length of crack slip, and $\Omega(\phi^*)$ is the intrinsic function of cohesive law containing information about the shape of cohesive law. Appendix A gives the explicit expressions of $\Omega(\phi^*)$ for some commonly-used cohesive laws.

Eq. (67) is available for constant normal pressure p_N and monotonic loading. For general loading conditions, the frictional cohesive law may be written in an incremental form. If there is no friction, i.e., $\tan \varphi = 0$, Eq. (67) degenerates to the parametric equation of cohesive law in our previous works (Feng et al., 2021; Feng and Li, 2022a,b, 2023b).

As an example, Fig. 4 gives the curve of exponential frictional cohesive law (See Appendix A for the detailed definition). As shown in the figure, the presence of friction leads to an increase in shear strength and also to the presence of residual stress, but does not change the shape of the cohesive law.

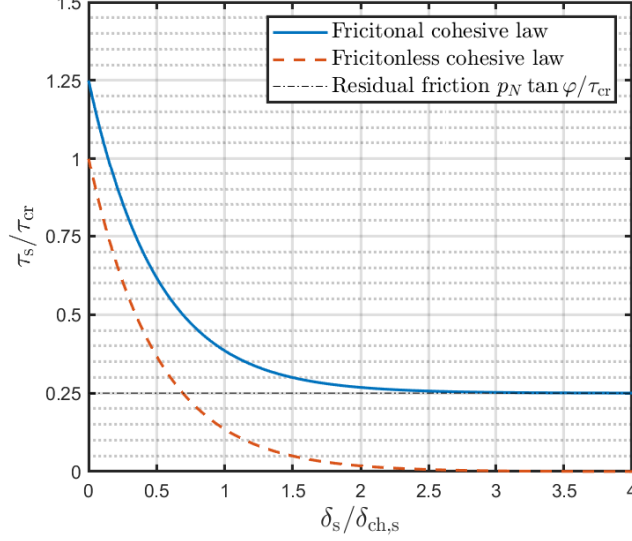


Figure 4: Exponential frictional cohesive law: Here, $p_N \tan \varphi = 0.25\tau_{cr}$.

4. Numerical algorithm and implementation

4.1. Three-field staggered algorithm and implementation

Theoretically, there are three field variables to be solved for: displacement $\mathbf{u}$, crack strain $\boldsymbol{\varepsilon}^c$, and phase-field ϕ . However, in the practice of numerical computation, it is more convenient to solve for $\{\mathbf{u}, \phi, \theta\}$ instead, where θ is the crack angle field. As will be demonstrated in Sec. 4.2, crack strain $\boldsymbol{\varepsilon}^c$ can be conveniently obtained in solving for displacement $\mathbf{u}$ using a return-mapping algorithm (Simo and Hughes, 2006).

This section gives the overall numerical algorithm of the proposed model, named the three-field staggered algorithm. The method for solving for displacement and crack angle will be given in Sec. 4.2 and Sec. 4.3, respectively.

Starting from the solution $\{\mathbf{u}_{i-1}, \phi_{i-1}, \theta_{i-1}\}$ at the $(i-1)$ -th time step, the three-field staggered algorithm at the i -th time step is described as follows.

- Initialization: Set $k = 0$ and $\{\mathbf{u}^{(k)}, \phi^{(k)}, \theta^{(k)}\} = \{\mathbf{u}_{i-1}, \phi_{i-1}, \theta_{i-1}\}$.
- Iteration $k = k + 1$:
 - Find $\mathbf{u}^{(k)} \in \mathcal{V}$ and with fixed $\{\phi, \theta\} = \{\phi^{(k-1)}, \theta^{(k-1)}\}$ such that $\forall \delta \mathbf{u} \in \bar{\mathcal{V}}$

$$\int_{\mathcal{B}} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}^{(k)}, \phi^{(k-1)}, \theta^{(k-1)}) : \nabla \delta \mathbf{u} \, d\mathbf{x} - \int_{\partial \mathcal{B}} \mathbf{t}_i^* \cdot \delta \mathbf{u} \, ds = 0, \quad (68)$$

where $\mathbf{t}_i^*$ is the specific loading at the i -th time step. The above equation is the standard weak form of the equilibrium condition in Eq. (32). In this substep, the crack strain $\boldsymbol{\varepsilon}^c$ is updated by the way. This process, as well as the specific expression of $\boldsymbol{\sigma}(\boldsymbol{\varepsilon}, \phi, \theta)$, is detailed in Sec. 4.2.

- Update $\theta^{(k)}$ explicitly based on $\{\mathbf{u}^{(k)}, \phi^{(k-1)}\}$ (see details in Sec. 4.3):

$$\theta^{(k)} = \Theta(\mathbf{u}^{(k)}, \phi^{(k-1)}). \quad (69)$$

- Find $\phi^{(k)} \in \mathcal{W}$ with fixed $\{\mathbf{u}, \theta\} = \{\mathbf{u}^{(k)}, \theta^{(k)}\}$ such that $\forall \delta\phi \in \overline{\mathcal{W}}$

$$\int_{\mathcal{B}} 2G_c \ell \nabla \phi^{(k)} \cdot \nabla \delta\phi \, d\mathbf{x} + \int_{\mathcal{B}} \left[\partial_{\phi} \psi_{\text{crack}}(\phi^{(k)}, \nabla \phi^{(k)}) - \mathcal{F}_{\text{driving}}(\boldsymbol{\varepsilon}^c{}^{(k)}, \phi^{(k)}) \right] \delta\phi \, dV \geq 0, \quad (70)$$

where the driving force is defined in Eq. (39) and Eq. (40). In simulations, we adopt Eq. (40) if $\phi \leq 1 \times 10^{-20}$ and Eq. (39) otherwise.

- End: Stop iteration when

$$\max \left(\|\mathbf{u}^{(k)} - \mathbf{u}^{(k-1)}\|, \|\phi^{(k)} - \phi^{(k-1)}\| \right) < \text{tol},$$

where $\|\cdot\|$ denotes the norm of variable and “tol” is some specific tolerance.

- Update: Set $\{\mathbf{u}_i, \phi_i, \theta_i\} = \{\mathbf{u}^{(k)}, \phi^{(k)}, \theta^{(k)}\}$.

Above, $\mathcal{V} = \{\mathbf{v} \in H^1(\mathcal{B}) : \mathbf{v} = \mathbf{u}_i^* \text{ on } \partial\mathcal{B}_u\}$ and $\overline{\mathcal{V}} = \{\mathbf{v} \in H^1(\mathcal{B}) : \mathbf{v} = \mathbf{0} \text{ on } \partial\mathcal{B}_u\}$ are the trial and test function spaces of displacement, respectively; $\mathcal{W} = \{w \in H^1(\mathcal{B}) : w_{i-1} \leq w \leq 1\}$ and $\overline{\mathcal{W}} = H^1(\mathcal{B})$ are the trial and test function spaces of phase-field, respectively. $H^1(\mathcal{B})$ is the Sobolev space containing functions v such that $|v|^2$ and $|\nabla v|^2$ are integrable over $\mathcal{B}$. Note that the irreversibility and boundedness of the phase-field variable are stressed in $\mathcal{W}$.

Numerical simulations of this work are implemented in FEniCS (Alnæs et al., 2015), an open-source finite element method platform. The weak form equations in (68) and (70) can be directly compiled using the Unified Form Language (UFL) in FEniCS. The irreversibility and boundedness conditions, $0 \leq \phi_{i-1} \leq \phi^{(k)} \leq 1$, can be conveniently guaranteed by the nonlinear optimization solver using the reduced space active set method included in the PETSc library (Balay et al., 2016).

4.2. Return-mapping algorithm with fixed crack angle

In the substep described in Eq. (68), as the crack angle is fixed, the stress can be conveniently obtained from the return-mapping algorithm without iteration, which is detailed as follows.

- **Elastic predictor:** Given $\boldsymbol{\varepsilon}_{i-1}^c$ and $\mathbf{u}$, calculate the trial stresses

$$\begin{aligned} \boldsymbol{\sigma}^{\text{trial}} &= \mathbb{E} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{i-1}^c), \\ \mathbf{q}^{\text{trial}} &= 2\mu \boldsymbol{\varepsilon}_{i-1}^c / [c_2 \omega(\phi)], \quad \mathbf{s}^{\text{trial}} = \boldsymbol{\sigma}^{\text{trial}} - \mathbf{q}^{\text{trial}}, \end{aligned} \quad (71)$$

where $\boldsymbol{\varepsilon}_{i-1}^c$ is the crack strain at the previous time step.

- **Plastic corrector:**

$$\begin{aligned} \boldsymbol{\sigma} &= \boldsymbol{\sigma}^{\text{trial}} - 2\mu \Delta \boldsymbol{\varepsilon}^c, \\ \boldsymbol{\varepsilon}^c &= \boldsymbol{\varepsilon}_{i-1}^c + \Delta \boldsymbol{\varepsilon}^c, \quad \Delta \boldsymbol{\varepsilon}^c = \frac{1}{2\mu} (1 - g_2(\phi)) \langle f^{\text{trial}} \rangle \mathbf{N}, \end{aligned} \quad (72)$$

where

$$\begin{aligned}
\mathbf{N} &= \frac{\sqrt{2}}{2} \text{sgn}(\sigma_{\alpha\beta}^{\text{trial}})(\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \\
f^{\text{trial}} &= \sqrt{2}F(\mathbf{s}^{\text{trial}}, \boldsymbol{\sigma}^{\text{trial}}, \mathbf{N}) = \mathbf{s}^{\text{trial}} : \mathbf{N} - \sqrt{2} \tan \varphi p_N^{\text{trial}}, \\
p_N^{\text{trial}} &= \langle -\boldsymbol{\sigma}^{\text{trial}} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \rangle.
\end{aligned} \tag{73}$$

The plastic corrector, Eq. (72), is derived by the following reasoning.

First, it is easy to check that if $F^{\text{trial}} \leq 0$ (or $f^{\text{trial}} \leq 0$), then the trial stresses in Eq. (71) satisfy all the governing equations in Eq. (65).

Second, if $F^{\text{trial}} > 0$ then $\Delta\boldsymbol{\varepsilon}^c > 0$ and thus it follows from Eq. (65) that

$$F = 0 \quad \Rightarrow \quad f = \mathbf{s} : \mathbf{N} - \sqrt{2} \tan \varphi p_N = 0, \tag{74}$$

where, with $\boldsymbol{\varepsilon}^c = \boldsymbol{\varepsilon}_{i-1}^c + \Delta\boldsymbol{\varepsilon}^c$,

$$\begin{aligned}
\boldsymbol{\sigma} &= \mathbb{E} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^c) = \boldsymbol{\sigma}^{\text{trial}} - 2\mu\Delta\boldsymbol{\varepsilon}^c \\
\mathbf{q} &= 2\mu\boldsymbol{\varepsilon}^c/[c_2\omega(\phi)] = \mathbf{q}^{\text{trial}} + 2\mu\Delta\boldsymbol{\varepsilon}^c/[c_2\omega(\phi)], \\
\mathbf{s} &= \boldsymbol{\sigma} - \mathbf{q} = \mathbf{s}^{\text{trial}} - 2\mu\Delta\boldsymbol{\varepsilon}^c/[1 - g_2(\phi)], \\
p_N &= \langle -\boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \rangle = \langle -(\boldsymbol{\sigma}^{\text{trial}} - 2\mu\Delta\boldsymbol{\varepsilon}^c) : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \rangle = p_N^{\text{trial}}.
\end{aligned} \tag{75}$$

In the derivation of Eq. (75) we have used $g_2(\phi) = 1/(1+c_2\omega(\phi))$, $\Delta\boldsymbol{\varepsilon}^c = \|\Delta\boldsymbol{\varepsilon}^c\|\mathbf{N}$, and $\mathbf{N} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = 0$.

Substituting Eq. (75) into Eq. (74), using $\Delta\boldsymbol{\varepsilon}^c = \|\Delta\boldsymbol{\varepsilon}^c\|\mathbf{N}$ and $\mathbf{N} : \mathbf{N} = 1$, we obtain

$$f = f^{\text{trial}} - 2\mu\|\Delta\boldsymbol{\varepsilon}^c\|/(1 - g_2(\phi)) = 0, \tag{76}$$

which implies

$$\|\Delta\boldsymbol{\varepsilon}^c\| = \frac{1}{2\mu}(1 - g_2(\phi))f^{\text{trial}}. \tag{77}$$

The above results are exactly what in Eq. (72) for the case where $f^{\text{trial}} > 0$.

Known from Eq. (72), with fixed crack angle and fixed phase-field, the problem reduces to a linear kinematic hardening problem where the stress $\boldsymbol{\sigma}$ can be written as an explicit function of $\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}_{i-1}^c$.

4.3. Algorithmic crack angle

Theoretically, the crack angle can be obtained from Eq. (61) if the stress state $\{\mathbf{s}, \boldsymbol{\sigma}\}$ is known. However, as shown in Eq. (72) the stress state can only be calculated if the crack angle is known. This dilemma implies a strongly nonlinear equation for the crack angle that can only be solved by some advanced iteration algorithm. Substituting Eq. (72) into Eq. (61) yields this nonlinear equation.

Fortunately, we find it is possible to write the crack angle as an explicit function of the trial state variables, such as $\boldsymbol{\sigma}^{\text{trial}}$ and $\mathbf{s}^{\text{trial}}$. These trial state variables only depend on strain $\boldsymbol{\varepsilon}$, phase-field ϕ , and the crack strain at the previous time step $\boldsymbol{\varepsilon}_{i-1}^c$. Therefore, one can update the crack angle explicitly based on $\{\mathbf{u}^{(k)}, \phi^{(k-1)}\}$ as stated in Eq. (69).

Let us denote by Θ the angle between the crack normal $\boldsymbol{\alpha}$ and the first principle direction of $\boldsymbol{\sigma}^{\text{trial}}$. The closed-form solution for Θ is derived as follows (see the derivation in [Appendix E](#)):

$$\Theta = \begin{cases} \Theta_1, & \sigma_{\alpha\alpha}^{\text{trial}}(\Theta_1) < 0, \\ \Theta_2, & \sigma_{\alpha\alpha}^{\text{trial}}(\Theta_2) > 0, \\ \Theta_3, & \text{otherwise,} \end{cases} \quad (78)$$

where $\sigma_{\alpha\alpha}^{\text{trial}}(\Theta) = \boldsymbol{\sigma}^{\text{trial}} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = a_{\sigma}^{\text{trial}} + r_{\sigma}^{\text{trial}} \cos(2\Theta)$, $a_{\sigma}^{\text{trial}} = (\sigma_1^{\text{trial}} + \sigma_2^{\text{trial}})/2$, $r_{\sigma}^{\text{trial}} = (\sigma_1^{\text{trial}} - \sigma_2^{\text{trial}})/2$, σ_1^{trial} and σ_2^{trial} are the first two principal values of $\boldsymbol{\sigma}^{\text{trial}}$,

$$\Theta_1 = \arcsin(C)/2 - \arctan(C_2/C_1)/2, \quad (79a)$$

$$\Theta_2 = -\text{sgn}(s_{\alpha\beta}^{\text{trial}})\pi/4 + \Theta_{s_1}^{\text{trial}}, \quad (79b)$$

$$\Theta_3 = -\text{sgn}(s_{\alpha\beta}^{\text{trial}}) \arccos(-a_{\sigma}^{\text{trial}}/r_{\sigma}^{\text{trial}})/2. \quad (79c)$$

Above, $\Theta_{s_1}^{\text{trial}}$ is the angle between the first principle direction of $\boldsymbol{s}^{\text{trial}}$ and the first principle direction of $\boldsymbol{\sigma}^{\text{trial}}$, $r_s^{\text{trial}} = (s_1^{\text{trial}} - s_2^{\text{trial}})/2$ where s_1^{trial} and s_2^{trial} are the first two principal values of $\boldsymbol{s}^{\text{trial}}$.

In Eq. (79a), the auxiliary parameters, C_1 , C_2 , and C , are defined as follows:

$$\begin{aligned} C_1 &= B - kA, \quad C_2 = A + kB, \\ C &= -\text{sgn}(C_1)ka_{\sigma}^{\text{trial}}(C_1^2 + C_2^2)^{-1/2} \tan \varphi, \end{aligned} \quad (80)$$

where

$$\begin{aligned} k &= \text{sgn}(s_{\alpha\beta}^{\text{trial}})(1 - g_2(\phi)) \tan \varphi, \\ A &= \text{sgn}(s_{\alpha\beta}^{\text{trial}})r_s^{\text{trial}} \cos(2\Theta_{s_1}^{\text{trial}}), \quad B = \text{sgn}(s_{\alpha\beta}^{\text{trial}})r_s^{\text{trial}} \sin(2\Theta_{s_1}^{\text{trial}}) + r_{\sigma}^{\text{trial}} \tan \varphi. \end{aligned} \quad (81)$$

Finally, the sign of $s_{\alpha\beta}^{\text{trial}}$ remains to determine to calculate the crack angle. It is proved in [Appendix E](#) that Θ should be in the range of $[-\pi/4, \pi/4]$. Based on this information, the sign of $s_{\alpha\beta}^{\text{trial}}$ can be determined from the following procedure:

We first assume that $\text{sgn}(s_{\alpha\beta}^{\text{trial}}) = -1$. If the calculated Θ is outside the range of $[-\pi/4, \pi/4]$, then we set $\text{sgn}(s_{\alpha\beta}^{\text{trial}}) = +1$ and calculate the crack angle again according to Eq. (78) and Eq. (79).

5. Numerical examples

5.1. Direct shear test

In the first example, we consider the direct shear test commonly encountered in geotechnical engineering. The purpose of this example is to test whether the presented model can correctly reproduce the shear strength enhancement and hysteresis loop caused by friction.

The geometry and boundary conditions are depicted in Fig 5. A displacement-controlled lateral shear load u_x^* is applied to the upper left side of the specimen, while a constant vertical pressure p_N is imposed on the top throughout the loading process. **In this example, the plane stress condition is adopted. That is, the out-of-plane stress component is assumed to be zero.**

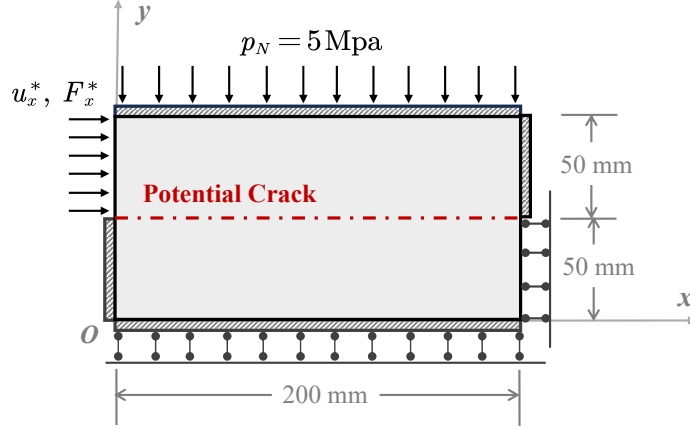


Figure 5: Geometry and boundary conditions of the direct shear test: Thickness of the specimen is set to be 1 mm. A specific description of some of the boundary conditions is given in Eq. (82).

For the sake of clarity, some displacement boundary conditions are listed as follows:

$$\begin{aligned}
 u_y &= 0, & (0 \leq x \leq L, y = 0), \\
 u_x &= 0, & (x = L, 0 \leq y \leq H/2), \\
 \partial u_y / \partial x &= 0, & (0 \leq x \leq L, y = H), \\
 \partial u_x / \partial y &= 0, & (x = 0, 0 \leq y \leq H/2) \cup (x = L, H/2 \leq y \leq H),
 \end{aligned} \tag{82}$$

where $L = 200$ mm and $H = 100$ mm.

The material parameters are chosen as follows: The fracture energy $G_c = 0.4$ N/mm, the inherent shear strength $\tau_{cr} = 3$ MPa, the Young's modulus $E = 3 \times 10^4$ MPa, the Poisson's ratio $\nu = 0.2$, and the friction angle $\varphi = 15^\circ$. The phase-field length scale $\ell = 1.5$ mm, resulting in a regularized crack with a width of about 15 mm. The cohesive law is set to be of the linearly decreasing type (Camacho and Ortiz, 1996). See Appendix A for the characteristic functions of the linear cohesive law. P1 triangular element and structured mesh are used in the simulation. The mesh size is fixed as 1 mm, nearly 1/15 of the phase-field crack width (see the subfigure in Fig. 6). To ensure the crack nucleates along the predefined path (the potential crack in Fig. 6), in this example (and only in this example) the crack normal α is enforced to be $[0, 1]^T$.

According to the loading fashion of u_x^* , two scenarios as follows are considered.

The first scenario is monotonic loading. That is, u_x^* is applied rightward and increased monotonically until the specimen fails due to the complete formation of a shear crack.

Fig. 6 gives the final crack pattern and the deformed configuration in the first scenario. As shown in the figure, the horizontal displacement u_x in the vicinity of the crack changes sharply, which is consistent with rigid slip along a fully developed cohesive crack. Fig. 7 gives the force-displacement response recorded at the loading surface for the first scenario. Fig. 7 also presents the crack patterns at three different loading levels. The results show that the proposed model can reproduce the typical phenomena induced by friction, such as the shear strength enhancement and residual friction force. We note that the peak forces are slightly larger than the theoretical value. This discrepancy is mainly induced by the nonuniform stress state in the specimen and the complex confinements on the boundary. A piece of evidence is shown in the top subfigure of Fig. 7: Two cracks nucleate simultaneously in the middle of the left and right sides of the specimen before the global peak load is reached, which clearly indicates that the stress is nonuniform. The result in Sec. 5.2 provides another piece of evidence: the peak load in a uniaxial compression test with a uniform stress state is in perfect agreement with the

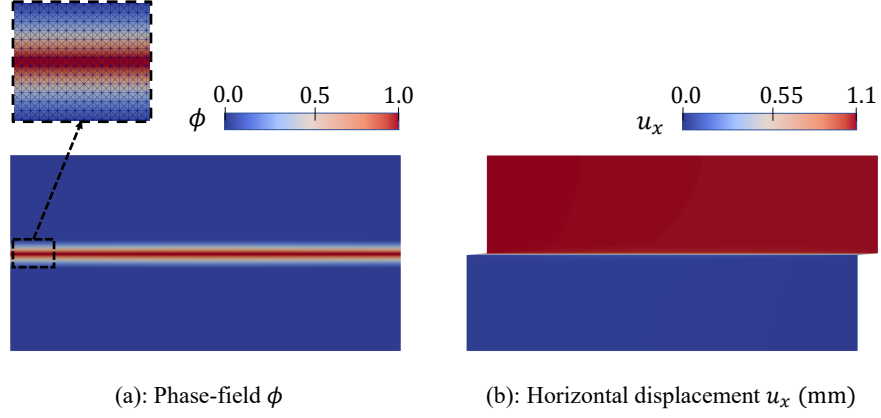


Figure 6: Final phase-field crack and deformed configuration in the first scenario: For visualization purposes, the deformation is magnified by a factor of 10.

theoretical result.

In the second scenario, we consider loading, unloading, and reverse-loading. Specifically, u_x^* is first applied rightward and increased monotonically until the cohesive-frictional shear crack develops to a certain level, and then u_x^* is reversed to the left until the specimen completely fails.

Fig. 8 presents the force–displacement hysteresis curve obtained in the second scenario. The result demonstrates the capability of the proposed model to reproduce typical plasticity-like behaviors induced by friction, such as residual deformation and reverse yielding. Fig. 8 also presents the crack patterns in the deformed configuration at several loading levels. For visualization purposes, the deformation is magnified by a factor of 50.

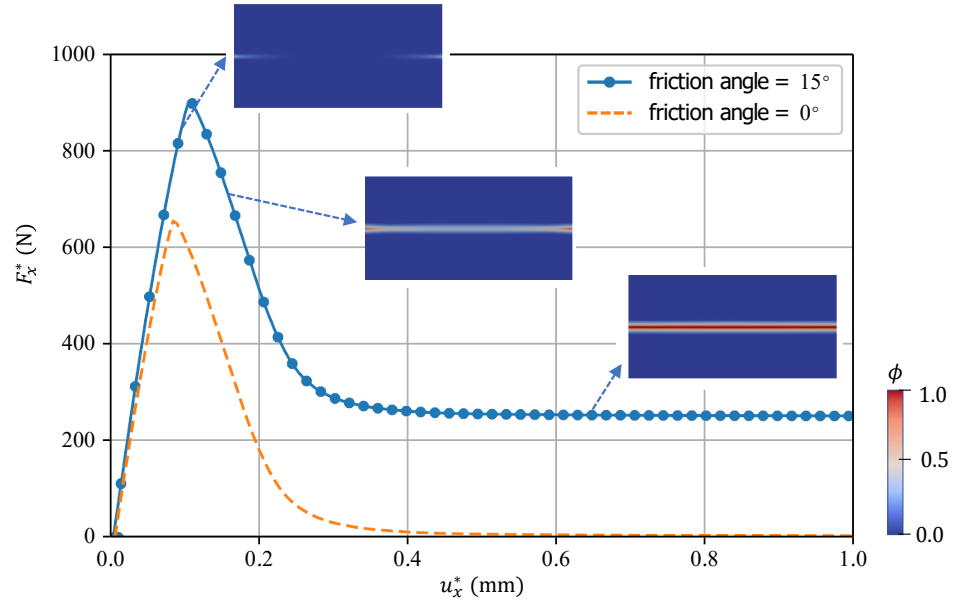


Figure 7: Force–displacement curve and phase-field cracks at different loading levels in the first scenario.

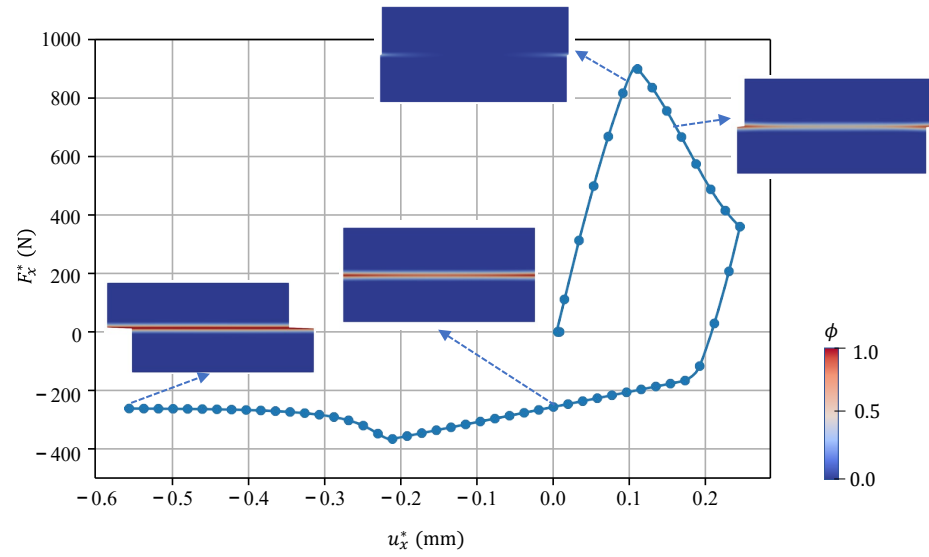


Figure 8: Force–displacement hysteresis curve and phase-field cracks at different loading levels in the second scenario.

5.2. Biaxial compression test

In this section, we consider **biaxial compression tests**. The purpose of this example is to test whether the proposed model can accurately capture the critical loading and nucleation angle in frictional fracture.

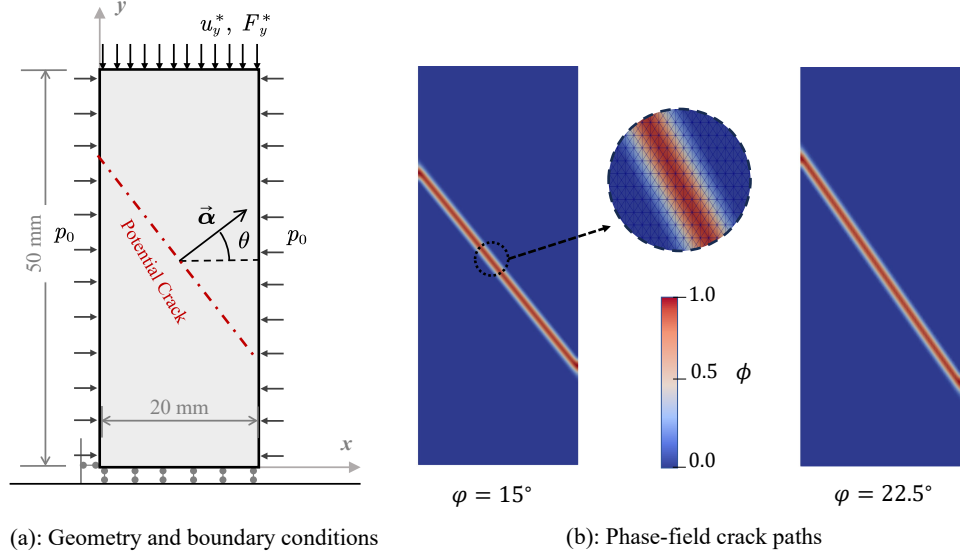


Figure 9: Geometry, boundary conditions, and phase-field crack in the uniaxial compression test with constant **confining** pressure: Thickness of the specimen is 1 mm. The theoretical value of θ is $\pi/4 - \varphi/2$, where φ is the friction angle.

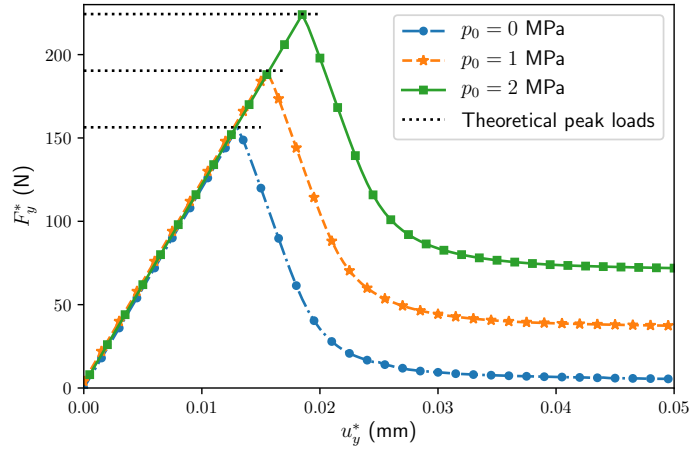


Figure 10: Force-displacement curves in the compression test with different **confining** pressure p_0 : The results are obtained using a fixed friction angle of 15° .

The geometry and boundary conditions are depicted in Fig. 9(a). A monotonically increasing displacement-controlled compressive load is imposed on the top of the specimen, whereas the vertical displacement of the bottom is fixed. During the loading process, the left and right sides of the specimen are subjected to a fixed compressive confining stress p_0 . **The plane stress assumption is adopted again. That is, the out-of-plane stress component is taken to be zero.**

The material parameters are chosen as follows: the fracture energy $G_c = 0.04$ N/mm, the inherent shear strength $\tau_{cr} = 3$ MPa, the Young's modulus $E = 3 \times 10^4$ MPa, the Poisson's ratio $\nu = 0.2$. Two different values of friction angle, $\varphi = 15^\circ$ and 22.5° , are considered, respectively. Linear cohesive law is

used and the phase-field length scale $\ell = 0.2$ mm, resulting in a phase-field crack width of about 2 mm. P1 triangular element and structured mesh are used. For accuracy, the mesh size should be fine enough to ensure that there are 5~10 **elements** in the phase-field crack band. In this example, the mesh size is set as 0.025 mm, nearly 1/8 of the width of the phase-field crack (see Fig. 9 (b)).

Fig. 9 (b) gives the phase-field crack paths in the simulation. The numerical crack angles θ 's are in perfect agreement with the Mohr-Coulomb's theoretical result, $\pi/4 - \varphi/2$. They are also consistent with our result in Eq. (61) for a uniform compressive stress state. Note that according to the Mohr-Coulomb theory, the crack nucleation angle is independent of the **confining** pressure p_0 as long as p_0 is not too large (at least the specimen should not be crushed directly by the **confining** pressure, e.g., $p_0 < 7.82$ Mpa if $\varphi = 15^\circ$).

Fig. 10 gives the force-displacement curves for different values of **confining** pressure. Based on the Mohr-Coulomb theory and a stress analysis on the critical plane (the potential crack in Fig. 9 (a)), the theoretical peak force can be derived as $(20 \text{ mm} \times 1 \text{ mm}) \times [\tau_{\text{cr}} + p_0(k + \tan \varphi)]/k$, where $k = (\cos \varphi + \tan \varphi \sin \varphi - \tan \varphi)/2$. As shown in Fig. 10, the peak loads predicted by the proposed phase-field model are in perfect agreement with the theoretical results. In addition, the phenomenon of residual friction force induced by p_0 is also captured by the proposed model. The shape of force-displacement curves are in good agreement with the results produced by linear cohesive law. The deviations at tails can be eliminated by using a very fine mesh. For a detailed convergence analysis with respect to mesh size in a phase-field cohesive fracture model, please refer to Section 7.3 of the work of Feng et al. (2021). The results in this example indicate that the proposed model has great potential in modeling the compression of quasi-brittle materials like concrete where the cohesive friction dissipation plays an important role at the end of loading stage (Ren et al., 2024a).

5.3. Slope stability problem

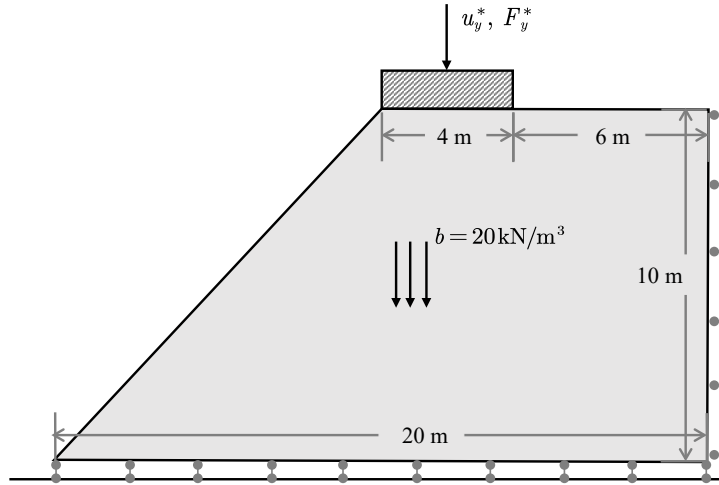
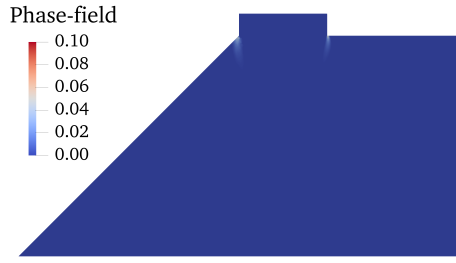
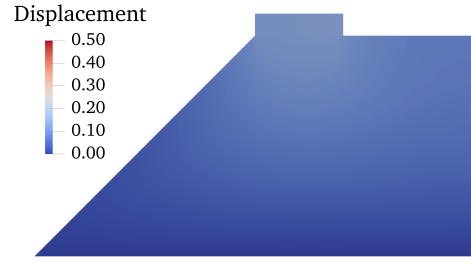


Figure 11: Geometry and boundary conditions of the slope stability problem: Thickness = 1 m. The top rectangle is a rigid foundation.

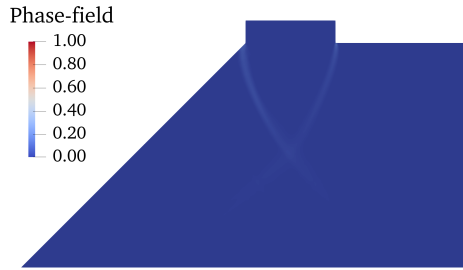
In this last example, we consider the slope stability problem typically encountered in soil mechanics. Specifically, we consider the problem firstly conjectured by Regueiro and Borja (2001), and later investigated by Haghighat and Pietruszczak (2015), Fei and Choo (2020) and Haghighat and Santillán (2023).



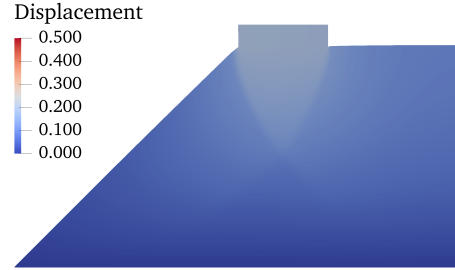
(a) Phase-field at $u_y^* = 0.06$ m



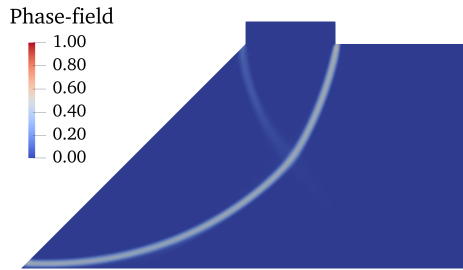
(b) Displacement at $u_y^* = 0.06$ m



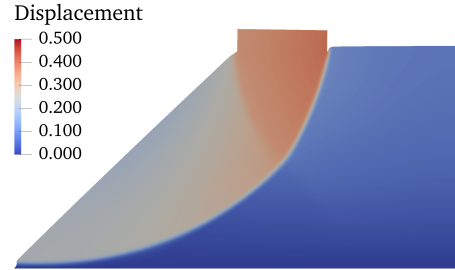
(c) Phase-field at $u_y^* = 0.10$ m



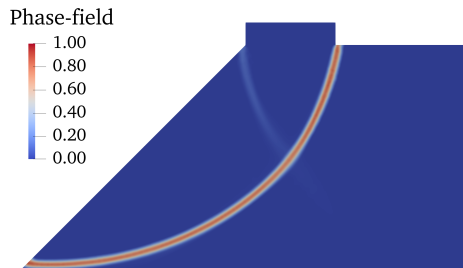
(d) Displacement at $u_y^* = 0.10$ m



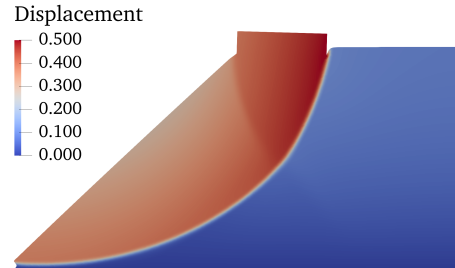
(e) Phase-field at $u_y^* = 0.25$ m



(f) Displacement at $u_y^* = 0.25$ m



(g) Phase-field at $u_y^* = 0.35$ m



(h) Displacement at $u_y^* = 0.35$ m

Figure 12: Crack pattern and deformation of the slope stability problem: In the right column, the deformed configurations are used, and the color indicates the magnitude of the displacement field, i.e., $\|\mathbf{u}\|$. The unit of displacement is m. $G_c = 12$ kJ/m².

The geometry and boundary conditions are depicted in Fig. 11. The slope is subjected to a gravitational body force of 20 kN/m^3 . In the simulation, gravity is first applied gradually in 10 time steps. Then a displacement-controlled compressive load is imposed on the top through a rigid foundation. The load increases monotonically until the slope loses stability due to the complete formation of a frictional-shear band.

The material parameters from the original work of Regueiro and Borja (2001) are adopted here: The inherent shear strength $\tau_{\text{cr}} = 40 \text{ kPa}$, the Young's modulus $E = 10 \text{ MPa}$, and the Poisson's ratio $\nu = 0.4$, and the friction angle $\varphi = 16.7^\circ$. The fracture energy was not given by Regueiro and Borja (2001) because it is not a necessary parameter in the plasticity model they considered. In our simulation, three values of fracture energy are considered: $G_c = 10, 11, 12 \text{ kJ/m}^2$ (or N/mm). Linear cohesive law is used and the phase-field length scale $\ell = 0.02 \text{ m}$, resulting in a phase-field crack width of about 0.2 m . Non-structured P1 triangular mesh is used. The characteristic mesh size is set at about 0.02 m .

Fig. 12 presents the evolution of phase-field and displacement field during the loading in the case of $G_c = 12 \text{ kJ/m}^2$. As expected, the slope fails due to the complete formation of a frictional-shear band. It is noteworthy that our model captures two crack nucleation paths from both ends of the rigid foundation. Then a wedge-like structure is formed. This result is consistent with the analysis in the works of Haghghat and Pietruszczak (2015) and Haghghat and Santillán (2023). This phenomenon was not captured by Fei and Choo (2020) because the crack angle θ was forced to be in the range of $[0, \pi/4]$ in their work. In comparison, our formulation does not need this constraint (see Eq. (61)).

According to the Mohr-Coulomb theory, the shear crack should be steeper than $\pi/4$ as shown in Fig. 12 due to the presence of friction (see also Fig. 9). This fact was not captured by the model of Haghghat and Santillán (2023). To improve computational efficiency, they used a simple deviatoric stress decomposition and did not explicitly consider the modeling of the crack angle. The resulting crack angle in their work can only be roughly $\pm\pi/4$.

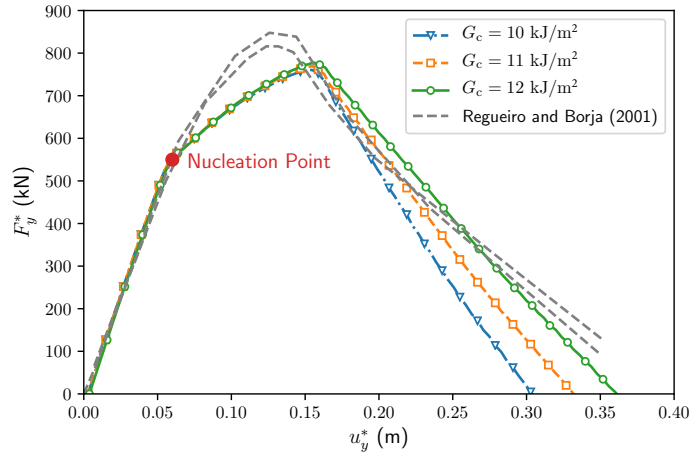


Figure 13: Force-displacement curves in the slope stability problem: The cracks nucleates at $u_y^* \approx 0.06 \text{ m}$. See Fig. 12a and Fig. 12b for the corresponding phase-field and displacement field at the nucleation point.

Fig. 13 gives the force-displacement responses for different values of G_c . The softening part of the curves is consistent with the linear cohesive law used in this example. Since a special algorithm was used to select the localization plasticity band in the original work of Regueiro and Borja (2001), only one crack nucleated from the right bottom of the foundation in their simulations, whereas two cracks nucleated in our simulations. This could be the reason for the deviation between the force-displacement responses from the nucleation point as shown in Fig. 13.

6. Summary and conclusion

This paper proposes a phase-field model for frictional-cohesive fracture. The model is derived based on two principles: the principle of energy conservation and an energetic stability condition termed the principle of inequality of virtual work. This work shows that all the governing equations, including the equilibrium condition, the phase-field crack evolution law, and even the yield condition and flow rule for frictional slip, can be derived from the aforementioned two principles alone.

The proposed model inherits the key property from our previous works (Feng et al., 2021; Feng and Li, 2023b): Using an integral transform, the information about the material's cohesive law is transformed into the energy density expression, which makes it possible to implement arbitrary forms of cohesive laws in the phase-field fracture theory.

Our theoretical and numerical results show that the presented model reflects the effect of Coulomb-type friction on fracture, including the enhancement of shear strength, frictional energy dissipation, and residual deformation. It is noteworthy that the proposed model can accurately describe not only the effect of friction on strength but also the effect of friction on the crack nucleation angle, faithfully consistent with the Mohr-Coulomb criterion.

In closing, we point out two directions for future research. First, the presented model can be extended to the general frictional mixed-mode fracture commonly encountered in geotechnical engineering. For example, it may be possible to use a small set of material parameters to reproduce the complex tensile wing cracks and shear cracks in the uniaxial compression tests on rocks with flaws (Wong and Einstein, 2009). The phenomenon of large differences in the tensile and shear strengths of materials such as rock and concrete can be explained directly by friction effects using the mixed-mode phase-field model.

Second, we note that the presented model is limited to a 2D setting. To extend the model to 3D problems, one may encounter an optimization problem concerning a crack surface normal vector rather than a scalar θ . This could dramatically increase the difficulty of the problem.

Acknowledgments

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Appendix A. Intrinsic functions $\omega(\phi)$ and $\Omega(\phi)$ for commonly-used cohesive laws

In this section, we list the explicit expressions of $\Omega(\phi^*)$ and $\omega(\phi)$ for some widely-used cohesive laws including the linear and exponential forms. Here we only consider the shear failure without friction. For mixed-mode fracture and other more complex cohesive laws, e.g. polynomial-type cohesive laws of arbitrary order, please refer to the original work of Feng et al. (2021).

Appendix A.1. Linear softening

The parametric equation set for the linear softening cohesive law is

$$\delta_s(\phi^*)/\delta_{ch,s} = \Omega(\phi^*) = \phi^* \quad \text{and} \quad \tau_s(\phi^*)/\tau_{cr} = 1 - \phi^*, \quad (\text{A.1})$$

where $\delta_{ch,s} = 2G_c/\tau_{cr}$ is the characteristic crack slip.

Substituting Eq. (A.1) into the integral transform Eq. (12) yields the intrinsic function $\omega(\phi)$ for linearly decreasing cohesive law:

$$\omega_{\text{linear}}(\phi) = \frac{1}{\pi^2(1-\phi)^2} \left(1 - (1-\phi)^2 \right). \quad (\text{A.2})$$

Appendix A.2. Exponential softening

The exponential softening cohesive law is

$$\tau_s(\delta_s) = \tau_{\text{cr}} \exp \left(-\frac{\tau_{\text{cr}} \delta_s}{G_c} \right), \quad (\text{A.3})$$

which can be expressed as the parametric equation set:

$$\delta_s(\phi^*)/\delta_{\text{ch},s} = \Omega(\phi^*) = -\frac{1}{2} \ln(1-\phi^*) \quad \text{and} \quad \tau_s(\phi^*)/\tau_{\text{cr}} = 1 - \phi^*. \quad (\text{A.4})$$

Substituting Eq. (A.4) into Eq. (12), one can obtain the following result after some mathematical manipulation (Feng et al., 2021):

$$\omega_{\text{exp}}(\phi) = \frac{1}{4\pi^2(1-\phi)^2} \operatorname{arctanh}^2 \left(\sqrt{1 - (1-\phi)^2} \right). \quad (\text{A.5})$$

Appendix B. Proof of the Kuhn-Tucker conditions

Let us consider the following variational inequality problem:

Find $\phi \in \mathcal{W}$ such that

$$\int_{\mathcal{B}} f(\phi, \nabla \phi) \delta \phi dV \geq 0 \quad \forall \delta \phi \in \bar{\mathcal{W}}_{\phi}, \quad (\text{B.1})$$

where $\mathcal{W} = \{w \in H^1(\mathcal{B}) : w \geq \phi_{i-1}\}$ and $\bar{\mathcal{W}}_{\phi} = \{w \in H^1(\mathcal{B}) : \text{there exists } h > 0 \text{ such that } \phi + hw \geq \phi_{i-1}\}$.

The irreversibility condition is stressed in the definitions of the sets $\mathcal{W}$ and $\bar{\mathcal{W}}$. If we let $f = \delta \mathcal{E} / \delta \phi$, then the problem in Eq. (33) is obtained.

At any point $\mathbf{x} \in \mathcal{B}$, we have the local form of Eq. (B.1) as follows:

Find $\phi \geq \phi_{i-1}$ such that

$$f(\phi, \nabla \phi) \delta \phi \geq 0 \quad (\text{B.2})$$

for all $\delta \phi$ that does not violate the irreversibility condition, $\exists h > 0 : \phi + h \delta \phi \geq \phi_{i-1}$.

Eq. (B.2) is a necessary and sufficient condition for Eq. (B.1). On the one hand, if we let $\delta \phi = 0$ everywhere except the infinitesimal region containing the point $\mathbf{x}$, then the condition Eq. (B.2) follows directly from Eq. (B.1). On the other hand, if Eq. (B.2) holds $\forall \mathbf{x} \in \mathcal{B}$, then clearly Eq. (B.1) holds as well.

In the following, we only consider the local form problem in Eq. (B.2).

Due to the unilateral constraint on $\delta \phi$, two cases as follows should be considered:

- Case 1: $\phi > \phi_{i-1}$. Namely, the potential optimum ϕ at some point $\mathbf{x}$ is larger than the phase-field at the previous time step.

In this case, since the magnitude $h > 0$ can be infinitely small, $\delta\phi$ can be positive or negative without violating the constraint $\phi + h\delta\phi \geq \phi_{i-1}$. Therefore, Inequality (B.2) holds only if $f(\phi, \nabla\phi) = 0$.

- Case 2: $\phi = \phi_{i-1}$ and thus $\dot{\phi} \propto (\phi - \phi_{i-1}) = 0$.

In this case, it follows from $h > 0$ and $\phi + h\delta\phi \geq \phi_{i-1}$ that $\delta\phi \geq 0$. Therefore Inequality (B.2) holds only if $f(\phi, \nabla\phi) \geq 0$.

The above results can be compactly written as the following conditions:

$$f\dot{\phi} = 0, \quad \dot{\phi} \geq 0 \quad \text{and} \quad f \geq 0, \quad (\text{B.3})$$

which are the widely-used Kuhn-Tucker conditions in constrained optimization.

Appendix C. Driving force at $\phi = 0$.

We assume that $0 < \omega(0) \ll 1$, the phase field, and crack strain $\boldsymbol{\varepsilon}^c$ at the previous time step are both equal to zero. In addition, we assume the crack normal vector $\boldsymbol{\alpha}$ is given.

According to Eq. (54), it is easy to find that if $|\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi < 0$, then $F = |s_{\alpha\beta}| - p_N \tan \varphi < 0$ and thus $\boldsymbol{\varepsilon}^c = d\boldsymbol{\varepsilon}^c = \mathbf{0}$. Therefore

$$\mathbf{q} = 2\mu\boldsymbol{\varepsilon}^c/[c_2\omega(\phi)] = \mathbf{0} \quad \text{if} \quad |\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi < 0. \quad (\text{C.1})$$

Now we consider the case where $|\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi \geq 0$ and $d\boldsymbol{\varepsilon}^c \neq 0$. It can be read from Fig. 3 or derived from $F = |s_{\alpha\beta}| - p_N \tan \varphi = 0$ that

$$\sigma_{\alpha\beta}(\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}) = \mathbf{q} + \mathbf{f}_N \quad (\text{C.2})$$

with $\mathbf{f}_N = \text{sgn}(\sigma_{\alpha\beta})p_N \tan \varphi(\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha})$.

Substituting $\boldsymbol{\sigma} = \mathbb{E} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^c) = \bar{\boldsymbol{\sigma}} - 2\mu\boldsymbol{\varepsilon}^c$, $\mathbf{q} = 2\mu\boldsymbol{\varepsilon}^c/[c_2\omega(\phi)]$ and $g(\phi) = 1/[1 + c_2\omega(\phi)]$ into Eq. (C.2) gives $\mathbf{q} = g_2(\phi)[\sigma_{\alpha\beta} - \text{sgn}(\sigma_{\alpha\beta})p_N \tan \varphi](\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha})$ and thus

$$\|\mathbf{q}\|^2 = \mathbf{q} : \mathbf{q} = 2g_2(\phi)^2(|\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi)^2 \quad \text{if} \quad |\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi \geq 0. \quad (\text{C.3})$$

Combing Eq. (C.1) and Eq. (C.3) and using the identity $g_2'(\phi) = -c_2\omega'(\phi)g(\phi)^2$, we have

$$\mathcal{F}_{\text{driving}} = -c_2\omega'(\phi)\frac{1}{2}\frac{\|\mathbf{q}\|^2}{2\mu} = g_2'(\phi)\frac{1}{2\mu}(|\bar{\sigma}_{\alpha\beta}| - p_N \tan \varphi)^2 \quad \text{if} \quad \phi = 0, \quad (\text{C.4})$$

which is the result of Eq. (40) in the main text.

Appendix D. Derivation procedure for crack angle in Eq. (61)

For the reader's convenience, the problem in Eq. (60) is restated here:

$$\theta = \arg \max_{-\pi/4 < \theta \leq \pi/4} F(\theta), \quad F(\theta) = |s_{\alpha\beta}| - p_N \tan \varphi \quad (\text{D.1})$$

Since $\boldsymbol{\alpha}$ is taken as the crack normal, then according to Eq. (23) we have $p_\alpha \leq p_\beta$ and hence $\sigma_{\alpha\alpha} \geq \sigma_{\beta\beta}$, which implies that $|\theta| \leq \pi/4$.

For the time being, we take θ the angle between a potential crack normal $\boldsymbol{\alpha}$ and the first principle direction of $\boldsymbol{\sigma}$. Using the Mohr's circle, stresses in Eq. (D.1) are expressed in terms of θ as follows:

$$s_{\alpha\beta} = -r_s \sin(2\theta - 2\theta_{s_1}), \quad (\text{D.2})$$

$$p_N = \langle -\sigma_{\alpha\alpha} \rangle, \quad (\text{D.3})$$

$$\sigma_{\alpha\alpha} = a_\sigma + r_\sigma \cos 2\theta, \quad (\text{D.4})$$

where $r_s = (s_1 - s_2)/2$, $a_\sigma = (\sigma_1 + \sigma_2)/2$, $r_\sigma = (\sigma_1 - \sigma_2)/2$, σ_1 and σ_2 are the first two principal values of $\boldsymbol{\sigma}$, s_1 and s_2 are the first two principal values of $\boldsymbol{s}$, and $\theta_{s_1} \in (-\pi/2, \pi/2]$ is the angle between the first principle direction of $\boldsymbol{s}$ and the first principle direction of $\boldsymbol{\sigma}$.

Due to the presence of Macaulay's brackets, three cases as follows should be considered.

Appendix D.1. Case 1: $\sigma_{\alpha\alpha} < 0$.

In this case, we have

$$F(\theta) = |-r_s \sin(2\theta - 2\theta_{s_1})| + (a_\sigma + r_\sigma \cos 2\theta) \tan \varphi. \quad (\text{D.5})$$

According to the value of θ_{s_1} , two subcases as follows should be considered:

Subcase 1.1: $\theta_{s_1} \in [0, \pi/4]$.

In this subcase, it is not difficult to check that $F(\theta_{s_1} + \Delta\theta) < F(\theta_{s_1} - \Delta\theta)$, where $\Delta\theta \in [0, \pi/4]$. In fact, $F(\theta_{s_1} + \Delta\theta) - F(\theta_{s_1} - \Delta\theta) = -2r_\sigma \sin 2\theta_{s_1} \sin 2\Delta\theta < 0$ as $\theta_{s_1} \in [0, \pi/4]$ and $\Delta\theta \in [0, \pi/4]$. Therefore, in this subcase the optimum θ should lie in $[-\pi/4, \theta_{s_1}]$. Thus $\sin(2\theta - 2\theta_{s_1}) \leq 0$ and the function $F(\theta)$ can be simplified as follows:

$$F(\theta) = -r_s \sin(2\theta - 2\theta_{s_1}) + (a_\sigma + r_\sigma \cos 2\theta) \tan \varphi. \quad (\text{D.6})$$

Letting $dF(\theta)/d(2\theta) = 0$, the optimum crack angle is obtained as:

$$\theta = -[\pi/4 - \arctan(A)/2], \quad A = \tan 2\theta_{s_1} + \tan(\varphi) r_\sigma / r_s / \cos 2\theta_{s_1}. \quad (\text{D.7})$$

Subcase 1.2: $\theta_{s_1} \in [-\pi/4, 0]$.

This subcase is symmetrical to Subcase 1.1. By the same reasoning, we can conclude that in this subcase, the optimum θ should lie in $[\theta_{s_1}, \pi/4]$ and the function $F(\theta)$ can be simplified as follows:

$$F(\theta) = +r_s \sin(2\theta - 2\theta_{s_1}) + (a_\sigma + r_\sigma \cos 2\theta) \tan \varphi. \quad (\text{D.8})$$

The maximizer of $F(\theta)$ can be obtained as:

$$\theta = \pi/4 - \arctan(A)/2, \quad A = -\tan 2\theta_{s_1} + \tan(\varphi) r_\sigma / r_s / \cos 2\theta_{s_1}. \quad (\text{D.9})$$

Subcase 1.3: $\theta_{s_1} \in (\pi/4, \pi/2]$.

By introducing an auxiliary variable

$$\theta_{s_1}^{\text{eff}} = \theta_{s_1} - \pi/2, \quad (\text{D.10})$$

the function $F(\theta)$ can be rewritten as follows:

$$F(\theta) = |r_s \sin(2\theta - 2\theta_{s_1}^{\text{eff}})| + (a_\sigma + r_\sigma \cos 2\theta) \tan \varphi, \quad (\text{D.11})$$

which is identical to Eq. (D.5) except that θ_{s_1} is replaced by $\theta_{s_1}^{\text{eff}}$.

Since $\theta_{s_1}^{\text{eff}} \in (-\pi/4, 0]$, this subcase should have the same optimum crack angle as that of Subcase 1.2 except for replacing θ_{s_1} by $\theta_{s_1}^{\text{eff}}$:

$$\theta = \pi/4 - \arctan(A)/2, \quad A = -\tan 2\theta_{s_1}^{\text{eff}} + \tan(\varphi) r_\sigma/r_s / \cos 2\theta_{s_1}^{\text{eff}}. \quad (\text{D.12})$$

Subcase 1.4: $\theta_{s_1} \in [-\pi/2, -\pi/4)$.

By introducing an auxiliary variable

$$\theta_{s_1}^{\text{eff}} = \theta_{s_1} + \pi/2, \quad (\text{D.13})$$

and using the same reasoning as in Subcase 1.3, we conclude that Subcase 1.4 should have the same optimum crack angle as that of Subcase 1.1 except for replacing θ_{s_1} by $\theta_{s_1}^{\text{eff}}$:

$$\theta = -[\pi/4 - \arctan(A)/2], \quad A = \tan 2\theta_{s_1}^{\text{eff}} + \tan(\varphi) r_\sigma/r_s / \cos 2\theta_{s_1}^{\text{eff}}. \quad (\text{D.14})$$

Summary of Case 1.

Summarizing the above results in Subcases 1.1~1.4, we find that the optimum angle can be written into a compact form

$$\theta = \theta_1 = -\text{sgn}(\theta_{s_1}^{\text{eff}}) [\pi/4 - \arctan(A)/2], \quad (\text{D.15})$$

where

$$\theta_{s_1}^{\text{eff}} = \theta_{s_1} - \text{sgn}(\theta_{s_1}) H(|\theta_{s_1}| - \pi/4) \pi/2, \quad (\text{D.16})$$

$H(\cdot)$ is the Heaviside step function, and

$$A = \text{sgn}(\theta_{s_1}^{\text{eff}}) \tan(2\theta_{s_1}^{\text{eff}}) + \tan(\varphi) r_\sigma/r_s / \cos(2\theta_{s_1}^{\text{eff}}). \quad (\text{D.17})$$

Now, the result of Eq. (62a) in the main text is obtained. The condition for Case 1 to occur is $\sigma_{\alpha\alpha}(\theta_1) < 0$.

Appendix D.2. Case 2: $\sigma_{\alpha\alpha} > 0$.

If $\sigma_{\alpha\alpha} > 0$, then $p_N = 0$ and thus

$$F(\theta) = |s_{\alpha\beta}| = |-r_s \sin(2\theta - 2\theta_{s_1})|. \quad (\text{D.18})$$

Using the auxiliary angle in Eq. (D.16), Eq. (D.18) can be rewritten as

$$F(\theta) = |s_{\alpha\beta}| = |r_s \sin(2\theta - 2\theta_{s_1}^{\text{eff}})|. \quad (\text{D.19})$$

The two possible maximizers are $\theta = \theta_{s_1}^{\text{eff}} \pm \pi/4$, where $\theta_{s_1}^{\text{eff}} \in [-\pi/4, \pi/4]$. If $\theta_{s_1}^{\text{eff}} > 0$, then $\theta = \theta_{s_1}^{\text{eff}} + \pi/4 > \pi/4$, which contradicts the condition $\theta \in [-\pi/4, \pi/4]$. Therefore, the maximizer $\theta = \theta_{s_1}^{\text{eff}} - \pi/4$ when $\theta_{s_1}^{\text{eff}} \in [0, \pi/4]$. Similarly, $\theta = \theta_{s_1}^{\text{eff}} + \pi/4$ when $\theta_{s_1}^{\text{eff}} \in [-\pi/4, 0)$.

In conclusion, the optimum angle in Case 2 is as follows:

$$\theta = \theta_2 = -\text{sgn}(\theta_{s_1}^{\text{eff}}) \pi/4 + \theta_{s_1}^{\text{eff}}. \quad (\text{D.20})$$

The condition for Case 2 to occur is $\sigma_{\alpha\alpha}(\theta_2) > 0$.

Appendix D.3. Case 3: $\sigma_{\alpha\alpha} = 0$.

The condition for this last case is an equality: $\sigma_{\alpha\alpha}(\theta) = a_\sigma + r_\sigma \cos 2\theta = 0$. Solving for θ gives

$$\theta = \theta_3 = -\text{sgn}(\theta_{s_1}^{\text{eff}}) \arccos(-a_\sigma/r_\sigma)/2, \quad (\text{D.21})$$

where the choice of the sign is made for consistency with Case 1 and Case 2. For example if $\theta_{s_1}^{\text{eff}} < 0$, then θ_1 , θ_2 and θ_3 are all in the range of $[0, \pi/4]$.

Appendix E. Derivation of the algorithmic crack angle in Eq. (78)

Here we demonstrate the derivation process for the case where $F^{\text{trial}} > 0$ and $p_N > 0$.

First we prove that $\text{sgn}(s_{\alpha\beta}) = \text{sgn}(s_{\alpha\beta}^{\text{trial}})$. Noting that $|s_{\alpha,\beta}| \propto \mathbf{s} : \mathbf{N} = \mathbf{s}^{\text{trial}} : \mathbf{N} - 2\mu\|\Delta\boldsymbol{\varepsilon}^c\|/(1 - g_2(\phi))$, $|s_{\alpha,\beta}| \geq 0$, and $2\mu\|\Delta\boldsymbol{\varepsilon}^c\|/(1 - g_2(\phi)) \geq 0$, we have $\mathbf{s}^{\text{trial}} : \mathbf{N} \geq 0$, which indicates that $\text{sgn}(s_{\alpha\beta}) = \text{sgn}(s_{\alpha\beta}^{\text{trial}})$.

Second we prove that $\Theta \in [-\pi/4, \pi/4]$, where Θ is the angle between the crack normal $\boldsymbol{\alpha}$ and the first principle direction of the trial stress $\boldsymbol{\sigma}^{\text{trial}}$. Since $\boldsymbol{\alpha}$ is defined as the crack normal, then it follows from Eq. (23) $\boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \leq \boldsymbol{\sigma} : (\boldsymbol{\beta} \otimes \boldsymbol{\beta})$ or $\theta \in [-\pi/4, \pi/4]$, where θ is the angle between the crack normal $\boldsymbol{\alpha}$ and the first principle direction of the real stress $\boldsymbol{\sigma}$. Note that

$$\boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = (\boldsymbol{\sigma}^{\text{trial}} - 2\mu\Delta\boldsymbol{\varepsilon}^c) : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = \boldsymbol{\sigma}^{\text{trial}} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}),$$

since $\Delta\boldsymbol{\varepsilon}^c : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = \|\Delta\boldsymbol{\varepsilon}^c\|\mathbf{N} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) = 0$ (see the definition of $\mathbf{N}$ in Eq. (55)). Similarly, we have $\boldsymbol{\sigma} : (\boldsymbol{\beta} \otimes \boldsymbol{\beta}) = \boldsymbol{\sigma}^{\text{trial}} : (\boldsymbol{\beta} \otimes \boldsymbol{\beta})$. Then it follows from $\boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \leq \boldsymbol{\sigma} : (\boldsymbol{\beta} \otimes \boldsymbol{\beta})$ that $\boldsymbol{\sigma}^{\text{trial}} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \leq \boldsymbol{\sigma}^{\text{trial}} : (\boldsymbol{\beta} \otimes \boldsymbol{\beta})$, which indicates $\Theta \in [-\pi/4, \pi/4]$.

Now we turn to the calculation of crack angle Θ . The key equation for the optimum crack angle is

$$R := \frac{\partial F}{\partial(2\theta)} = 0, \quad (\text{E.1})$$

where F is the yield surface function given in Eq. (47).

In the most complex scenario where $p_N > 0$, we have

$$F(\boldsymbol{\sigma}, \mathbf{s}, \theta) = \frac{\sqrt{2}}{2} \mathbf{s} : \mathbf{N} + \boldsymbol{\sigma} : (\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) \tan \varphi \quad (\text{E.2})$$

and

$$R(\boldsymbol{\sigma}, \mathbf{s}, \theta) = \frac{\sqrt{2}}{2} \mathbf{s} : \mathbf{M} + \text{sgn}(s_{\alpha\beta}) \frac{\sqrt{2}}{2} \boldsymbol{\sigma} : \mathbf{N}, \quad (\text{E.3})$$

where

$$\mathbf{N} = \frac{\sqrt{2}}{2} \text{sgn}(s_{\alpha\beta}) (\boldsymbol{\alpha} \otimes \boldsymbol{\beta} + \boldsymbol{\beta} \otimes \boldsymbol{\alpha}), \quad \mathbf{M} = \frac{\partial \mathbf{N}}{\partial 2\theta} = \frac{\sqrt{2}}{2} \text{sgn}(s_{\alpha\beta}) (\boldsymbol{\beta} \otimes \boldsymbol{\beta} - \boldsymbol{\alpha} \otimes \boldsymbol{\alpha}). \quad (\text{E.4})$$

In the above derivation, we have used $d\boldsymbol{\alpha}/d\theta = \boldsymbol{\beta}$ and $d\boldsymbol{\beta}/d\theta = -\boldsymbol{\alpha}$ (use $\boldsymbol{\alpha} = [\cos \theta, \sin \theta]^T$ and $\boldsymbol{\beta} = [-\sin \theta, \cos \theta]^T$ for the proof).

In addition, the following orthogonality conditions will prove useful:

$$(\boldsymbol{\alpha} \otimes \boldsymbol{\alpha}) : \mathbf{N} = 0, \quad \mathbf{N} : \mathbf{M} = 0, \quad (\text{E.5})$$

Using the relations in Eq. (75) and Eq. (E.5), F and R can be rewritten in terms of trial stresses as follows:

$$F = F^{\text{trial}} - \frac{2\mu}{1 - g_2(\phi)} \Delta\lambda, \quad (\text{E.6a})$$

$$R = R^{\text{trial}} - 2\mu \text{sgn}(s_{\alpha\beta}) \tan \varphi \Delta\lambda, \quad (\text{E.6b})$$

where $F^{\text{trial}} = F(\boldsymbol{\sigma}^{\text{trial}}, \mathbf{s}^{\text{trial}}, \theta)$ and $R^{\text{trial}} = R(\boldsymbol{\sigma}^{\text{trial}}, \mathbf{s}^{\text{trial}}, \theta)$.

Substituting Eq. (E.6) into Eq. (E.1) gives the following key condition:

$$R^{\text{trial}} - kF^{\text{trial}} = 0, \quad (\text{E.7})$$

where, for convenience, we have introduced an auxiliary parameter:

$$k = (1 - g_2(\phi)) \text{sgn}(s_{\alpha\beta}) \tan \varphi. \quad (\text{E.8})$$

Using the Mohr's circle, F^{trial} and R^{trial} can be expressed in terms of Θ as follows:

$$F^{\text{trial}} = -\text{sgn}(s_{\alpha\beta}^{\text{trial}}) \sin(2\Theta - 2\Theta_{s_1}^{\text{trial}}) + r_{\sigma}^{\text{trial}} \tan \varphi \cos 2\Theta + a_{\sigma}^{\text{trial}} \tan \varphi, \quad (\text{E.9a})$$

$$R^{\text{trial}} = -\text{sgn}(s_{\alpha\beta}^{\text{trial}}) \cos(2\Theta - 2\Theta_{s_1}^{\text{trial}}) - r_{\sigma}^{\text{trial}} \tan \varphi \sin 2\Theta, \quad (\text{E.9b})$$

where, as explained in the main text, $\Theta_{s_1}^{\text{trial}}$ is the angle between the first principle direction of $\mathbf{s}^{\text{trial}}$ and the first principle direction of $\boldsymbol{\sigma}^{\text{trial}}$; $a_{\sigma}^{\text{trial}}$ and $r_{\sigma}^{\text{trial}}$ are the average stress and “radius” of $\boldsymbol{\sigma}^{\text{trial}}$; and r_s^{trial} is the “radius” of $\mathbf{s}^{\text{trial}}$.

Substituting Eq. (E.9) into Eq. (E.7) and using the sum and difference formulas of triangle functions, we have the following result after some rearrangement:

$$|C_1| \sin 2\Theta + \text{sgn}(C_1) C_2 \cos 2\Theta = -\text{sgn}(C_1) k a_{\sigma}^{\text{trial}} \tan \varphi, \quad (\text{E.10})$$

where the auxiliary parameters, C_1 and C_2 , are given in Eq. (80).

Eq. (E.10) can be further simplified as

$$\sin(2\Theta + \Theta^*) = C, \quad (\text{E.11})$$

where, as given in Eq. (80),

$$C = -\text{sgn}(C_1) k a_{\sigma}^{\text{trial}} (C_1^2 + C_2^2)^{-1/2} \tan \varphi, \quad (\text{E.12})$$

and

$$\Theta^* = \arctan(C_2/C_1) \quad (\text{E.13})$$

Solving Eq. (E.11) gives

$$\Theta = \frac{1}{2} \arcsin C - \frac{1}{2} \arctan(C_2/C_1) \quad (\text{E.14})$$

which is the result in Eq. (79a).

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