Numerical simulation of mixed mode (I and II) fracture behavior of pre-cracked rock using the strong discontinuity approach

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7 Abstract

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The existence of macroscopic flaws in geomaterial structures profoundly influences their load-carrying capacity and failure patterns. This paper is devoted to the numerical investigation of mixed mode fracture propagation in a cracked Brazilian disk (CBD) specimen by means of the embedded strong discontinuity approach (SDA). A recently modified nonassociated, three-invariant cap plasticity model with mixed isotropic/kinematic hardening is used to predict the continuum response for the intact part of the specimen. In addition, this constitutive model adopts bifurcation analysis to track the inception of new localization and crack path propagation. For the post-localization regime, a cohesive-law fracture model, able to address mixed-model failure condition, is implemented to characterize the constitutive softening behavior on the surface of discontinuity. To capture propagating fracture, the Assumed Enhanced Strain (AES) method is employed. Furthermore, particular mathematical treatments are incorporated into the simulation concerning numerical efficiency and robustness issues. Finally, the results obtained from the enhanced FE simulations are analyzed and critically compared with experimental results available in the literature.

8 Keywords: Fracture; Strong discontinuities; Cap plasticity; Bifurcation analysis; Crack propagation

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9 1. Introduction

Numerical simulation of geotechnical and geological structures, especially 10 in the platform of the finite element (FE) method, has attracted much re-11 search interest with the advent of modern computational resources. One cru-12 cial part of an FE simulation is the selection of an appropriate constitutive 13 material model, since geomaterials can exhibit many complex and interact-14 ing behaviors. At low confining pressure, localized deformation in the form 15 of shear and/or dilation bands or fractures may occur due to the growth 16 and coalescence of micro-cracks and pores. At high confining pressure, on 17 the contrary, delocalized irreversible deformation may occur in the form of 18 shear-enhanced compaction. The latter response, generally accompanied by 19 material hardening, is the result of pore collapse, grain crushing, internal 20 locking and other microphysical mechanisms. 21

Further compounding the complexity of this response, these materials 22 typically contain macroscopic inhomogeneities such as natural flaws, cracks, 23 joint sets, and bedding planes. The existence of macro-structural hetero-24 geneities in geo-systems renders them vulnerable to catastrophic failures at 25 drastically lower loads than those expected for intact structures. Brittle 26 faulting can be triggered from these zones and propagate under crack open-27 ing (mode I), sliding (mode II) or a mixture of modes. Notably, in gravity 28 dams most of the observed cracks are mixed mode (Kishen and Singh (2001); 29 Roth et al. (2015)), and hydraulic fractures propagate in mixed-mode condi-30 tions from the walls of wellbores (Rahman et al. (2002)). 31

Over the past decades, multiple laboratory tests with different config-32 urations (including circular disc (Al-Shayea (2005); Erarslan and Williams 33 (2012)), semi-circular disc(Aliha et al. (2010); Aliha and Ayatollahi (2013)), 34 round bar, and rectangular-beam (Rinehart et al. (2015))) have been designed 35 to investigate the mixed-mode fracture behavior in geomaterials. Among 36 these tests is the cracked Brazilian disc (CBD) specimen, which has been 37 frequently utilized for rock materials due to the amenity of test specimen 38 preparation from the rock cores. Other reasons in adopting the CBD speci-39 men include the relatively straightforward test procedure with regard to the 40 application of compressive rather than tensile load and the capability to eas-41 ily replicate various combinations of mode I and II fracture propagation by 42 varying the initial crack inclination angle relative to the applied load. 43

For many applications, mixed-mode fracture in rocks has been simplified 44 to empirical approaches (Yao (2012); Jaeger et al. (2009)) or linear elastic 45 fracture mechanics (LEFM). In these approaches conventional fracture the-46 ories (such as the maximum tangential stress criterion (MTS) (Erdogan and 47 Sih(1963)), the minimum strain energy density criterion Sih(1974), the max-48 imum energy release rate criterion (Hussain et al. (1974))) have been used to 49 predict resistance to and direction of the fracture growth. However, LEFM 50 is not always applicable to geomaterials (see, e.g. Rubin (1993)), and other 51 more advanced methods are often computationally challenging to implement. 52 In the case of quasi-brittle materials, cohesive zone models, which may be 53 traced to the pioneering work of Dugdale (1960) and Barenblatt (1962), are 54

an appropriate alternatives to describe the micromechanical features under-55 lying the evolution of damage in the FPZ. These models interpret the FPZ 56 as an interface along which the displacement jump is related to transfer-57 ring cohesive tractions. Cohesive zone models have been proposed in various 58 settings (see Park and Paulino (2013) for a review of models), but the best 59 known are the potential-based laws by Tvergaard (1990) and Xu and Needle-60 man (1993) and the linear laws by Camacho and Ortiz (1996) and Ortiz and 61 Pandolfi (1999). 62

The numerical simulation of crack growth within the finite element method 63 may be carried out with different techniques. One early approach is discrete-64 crack model employing interface elements so that the crack is allowed to prop-65 agate along the boundaries of the finite elements. Though several attempts 66 have been made in a case of crack paths unknown a priori to generate robust 67 and reliable tools for automatic remeshing procedure (see, for example, Ma-68 ligno et al. (2010); Boussetta et al. (2006)), discrete-crack models still suffer 69 from some shortcomings, such as spurious stress transferring across crack sur-70 faces and mesh bias. To alleviate these numerical difficulties, fine meshes are 71 needed, which lead to large-scale and in computationally expensive systems. 72 In recent years, models with cracks embedded in finite elements including 73 either nodal enrichment, the eXtended or Generalized finite element method 74 (XFEM or GFEM) (Gupta et al. (2015); Wu et al. (2015); Shen and Lew 75 (2014); Kramer et al. (2013); Chen et al. (2012); Belytschko et al. (2001)), or 76 elemental enrichment, the Embedded finite element method (EFEM) (Weed 77

et al. (2015); Zhang et al. (2015); Linder and Zhang (2014); Wu (2011); Foster 78 et al. (2007); Borja and Regueiro (2001); Armero and Garikipati (1996); Simo 79 et al. (1993)) have been applied successfully to simulation of fracture propa-80 gation. A comparative study by Oliver et al. (2006b) showed that EFEM is 81 computationally more efficient than XFEM, though it cannot accurately cap-82 ture the crack tip stresses. In addition, by focusing on slip patterns, Borja 83 (2008) has elucidated that the extended FE solutions require higher-order 84 crack tip enhancement in order to fully capture the strain singularity at the 85 crack tip and EFEM could predict larger slip (i.e., softer response) compared 86 to the XFEM solutions otherwise. Due to some of the appealing features of 87 the EFEM, computational efficiency being a primary one, we have chosen to 88 adopt this method for the simulation of mixed-mode fracture in CBDs. 89

The remainder of this paper is organized as follows: Section 2 reviews a 90 recently modified cap plasticity model for geomaterials. In Section 3 first, 91 the kinematics of a strong discontinuity are outlined. Second, to capture 92 the fracture initiation and its orientation, bifurcation theory is reviewed. At 93 the end of Section 3, a cohesive fracture model is summarized to describe 94 evolution of the damage with either coupled opening/sliding displacements 95 or solely frictional slip mode. In Section 4, the finite element approximation 96 using assumed enhanced strain (AES) method is briefly discussed. The nu-97 merical implementation of the models for both strain hardening and softening 98 responses is given in Section 5. In Section 6, the numerical efficiency and 99 robustness of both constitutive model and post-localization model are briefly 100

discussed. Finally, Section 7 describes a benchmark example of a CBD specimen to investigate the mixed mode fracture behavior of pre-cracked limestone
rock, and the finite element solutions are compared with experimental results.

¹⁰⁴ 2. Three-invariant isotropic kinematic hardening cap plasticity model

Even though recently various multiscale computational approaches (see for example Tonge and Ramesh (2016); Flores et al. (2015); Oliver et al. (2015); Liu et al. (2015); Cusatis et al. (2014)) have been developed, investigating some micromechanical features of complex geomaterials, continuum plastic constitutive models are still the most widely acknowledged method to capture material nonlinearities and inelastic behaviors.

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Cap plasticity models typically utilized in the modeling of complex me-112 chanical behavior of porous geomaterials capture shear yielding at low mean 113 stress and inelastic compaction at higher mean stress. These models can take 114 into account one or more other aspects such as pressure-sensitive yielding, 115 differences in strength in triaxial compression and extension, dilatancy and 116 the Baushinger effect, among others. In this section, the formulation and 117 numerical implementation of a nonassociated, three-invariant, isotropic and 118 kinematic hardening cap plasticity model are briefly described. The model 119 comprises a pressure-dependent shear yield surface, hardening compaction 120 cap and newly added elliptical tension cap as shown in Fig. 1. For more 121 details and motivation of the model, the reader is referred to Motamedi and 122

Foster (2015).



Figure 1: Cap plasticity model: three dimensional view of the yield surface (the exterior free mesh surface) and plastic potential surface (the interior blue solid) in principal stress space.

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124 2.1. Yield functions and plastic potentials

Assuming that the yielding behavior is isotropic, the yield function f and 125 plastic potential function g can be expressed in terms of stress invariants 126 (e.g. I_1, J_2 and J_3). In the case of kinematic hardening, a deviatoric backstress 127 tensor α is presented to capture the Bauschinger effect, such that the relative 128 stress tensor can be defined as $\boldsymbol{\xi} = \boldsymbol{\sigma} - \boldsymbol{\alpha}$. Given a back stress with an 129 appropriate translation rule (Foster et al. (2005)), the yielding of the material 130 may be expressed in terms of invariants of the relative stress $(I_1, J_2^{\xi} \text{ and } J_3^{\xi})$. 131 Many cap plasticity models have been proposed, for example Lu and 132 Fall (2015); Gamnitzer and Hofstetter (2015); DorMohammadi and Khoei 133 (2008); Kohler and Hofstetter (2008); Grueschow and Rudnicki (2005). In 134 this work, we follow a smooth cap formulation initially proposed by Fossum 135

and Brannon (2004). The yield function f and conjugated plastic potential ₁₃₇ g take the following form:

$$f = \Gamma(\beta^{\xi})\sqrt{J_2^{\xi}} - \sqrt{F_c}(F_f - N)$$
(2.1)

$$g = \Gamma(\beta^{\xi})\sqrt{J_2^{\xi}} - \sqrt{F_c^g}(F_f^g - N)$$
(2.2)

where the material parameter N indicates the maximum allowed translation of the initial yield surface during kinematic hardening and Γ accounts for the difference in triaxial extension vs. compression strength. The Lode angle β^{ξ} is the function of second and third invariants of the deviatoric relative stress dev ξ . The exponential shear failure function F_f and the corresponding plastic potential surface F_f^g are given as

$$F_f(I_1) = A - C \exp(B I_1) - \theta I_1$$
 (2.3)

$$F_f^g(I_1) = A - C \exp(L I_1) - \phi I_1 \tag{2.4}$$

The shear failure surface F_f captures the pressure dependence of the shear strength of the material where A, B, C and θ are all non-negative material parameters determined from peak stress experimental data, using a procedure described in (Fossum and Brannon (2004)). L and ϕ are determined from experimental measurements of volumetric plastic deformation. The cap function F_c generates two smooth elliptical caps to the yield function in both tensile and compressive stress zones. This function couples hydrostatic and deviatoric stress-induced deformation of the material. The cap function F_c and the corresponding one for plastic potential F_c^g are formulated as

$$F_c(I_1,\kappa) = 1 - H(\kappa - I_1) \left(\frac{I_1 - \kappa}{X(\kappa) - \kappa}\right)^2 - H(I_1 - I_1^T) \left(\frac{I_1 - I_1^T}{3T - I_1^T}\right)^2 (2.5)$$

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$$F_c^g(I_1,\kappa) = 1 - H(\kappa - I_1) \left(\frac{I_1 - \kappa}{X^g(\kappa) - \kappa}\right)^2 - H(I_1 - I_1^T) \left(\frac{I_1 - I_1^T}{3T - I_1^T}\right)^2 (2.6)$$

where κ stands for the branch point in which combined porous/microcracked yield surface deviates from the nonporous profile for full dense bodies. The function $X(\kappa)$ is the intersection of the cap surface with the I_1 axis in the $\sqrt{J_2}$ versus I_1 plane and signifies the position at which pressure under pure hydrostatic loading would be sufficient to prompt grain crushing and pore collapse mechanisms.

Furthermore, this plasticity model is furnished with two internal variables, α and κ . The translational back stress tensor α is adopted to capture kinematic hardening. Additionally, on the cap surface, κ is a scalar isotropic hardening parameter, which allows the yield surface to isotropically expand. The combined isotropic/kinematic hardening of the cap model is visualized by the schematic diagram in Fig. 3. The description of evolution laws for



Figure 2: Two-dimensional representation of yield and potential surfaces in meridional stress space; deviatoric stress $\sqrt{J_2}$ versus mean stress I_1 .

- ¹⁶⁶ isotropic/kinematic hardening parameters and their correspondence with mi-
- ¹⁶⁷ crostructural deformations are discussed in Motamedi and Foster (2015).



Figure 3: Three dimensional view of initial yield surface (the interior gray solid) evolution in principal stress space for: (a) isotropic hardening and (b) mixed isotropic-kinematic hardening.

¹⁶⁸ 2.2. Generalized Hooke's law and flow rule

The generalized Hooke's law for linear isotropic elasticity can be writtenas:

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{C}^e : \dot{\boldsymbol{\epsilon}}; \ \boldsymbol{C}^e = \lambda \mathbf{1} \otimes \mathbf{1} + 2\mu \boldsymbol{I}$$
(2.7)

where **1** is the second order identity tensor, I is the fourth-order symmetric identity tensor, λ and μ are the Lamé parameters and C^e is the fourth-order isotropic elasticity tensor. For infinitesimal strain, an additive decomposition of the total strain rate $\dot{\epsilon}$ into the elastic and plastic parts is introduced

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^e + \dot{\boldsymbol{\epsilon}}^p \tag{2.8}$$

A non-associative flow rule is assumed for plastic flow as below

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\gamma} \frac{\partial g}{\partial \boldsymbol{\sigma}} \tag{2.9}$$

In addition, the continuum elasto-plastic tangent C^{ep} can be derived as the following

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{C}^{ep} : \dot{\boldsymbol{\epsilon}}; \ \boldsymbol{C}^{ep} = \left(\boldsymbol{C}^{e} - \frac{1}{\chi}\boldsymbol{C}^{e} : \frac{\partial g}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial f}{\partial \boldsymbol{\sigma}} : \boldsymbol{C}^{e}\right)$$
(2.10)

178 in which

$$\chi = \frac{\partial f}{\partial \boldsymbol{\sigma}} : \boldsymbol{C}^{e} : \frac{\partial g}{\partial \boldsymbol{\sigma}} - \frac{\partial f}{\partial \boldsymbol{\alpha}} : \boldsymbol{h}^{\boldsymbol{\alpha}} - \frac{\partial f}{\partial \kappa} h^{\kappa}$$
(2.11)

179 3. Strong discontinuity:

180 3.1. Kinematics and governing equations

For strong discontinuities, the displacement field experiences a spatial jump $\llbracket \boldsymbol{u} \rrbracket = \boldsymbol{u}^+ - \boldsymbol{u}^-$ across the material surface *S* separating the subdomains Ω^- and Ω^+ of an otherwise continuous body Ω , see Fig. 4. The displacement ¹⁸⁴ field in the context of strong discontinuity kinematics is given by

$$\boldsymbol{u}\left(\boldsymbol{x},t\right) := \underbrace{\bar{\boldsymbol{u}}\left(\boldsymbol{x},t\right)}_{continuious \ part} + \underbrace{\left[\!\left[\boldsymbol{u}(t)\right]\!\right] H_{S}\left(\boldsymbol{x}\right)}_{jump \ discontinuity}$$
(3.1)

in which $H_{S}(\boldsymbol{x})$ is the Heaviside function across the surface defined by the conditions

$$H_{S}(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \Omega^{+} \\ 0 & \text{if } \boldsymbol{x} \in \Omega^{-} \end{cases}$$
(3.2)



Figure 4: Body Ω with planar strong discontinuity S fixed at the reference configuration, $(\Omega = \Omega^+ \cup \Omega^- \cup S, \ \Gamma = \Gamma^t \cup \Gamma^g)$

In this study, it is assumed that the jump discontinuity $\llbracket u \rrbracket$ is piecewise constant along surface S (i.e. independent of x) so that the gradient $\nabla \llbracket u \rrbracket$ is ignored. The total strain rate tensor resulting from this field is the symmetric component of the displacement gradient tensor, which can be derived in ¹⁹¹ compact form as below

$$\dot{\boldsymbol{\epsilon}} := \underbrace{\operatorname{sym}(\nabla \dot{\boldsymbol{u}})}_{regular \ part} + \underbrace{\operatorname{sym}\left(\left[\dot{\boldsymbol{u}}\right] \otimes \boldsymbol{n}\right) \delta_S}_{singular \ part}$$
(3.3)

where \boldsymbol{n} is the unit normal vector to the surface S and pointing in the direction of Ω^+ . The Dirac delta distribution δ_s indicates unbounded strain at the discontinuity interface.

The local form of quasi-static, isothermal equilibrium for a body with strong discontinuity leads to the following set of governing equations

$$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b} = \boldsymbol{0} \text{ in } \Omega \tag{3.4a}$$

$$\boldsymbol{\sigma} \cdot \boldsymbol{\nu} = \boldsymbol{t}^{\boldsymbol{\sigma}} \text{ on } \boldsymbol{\Gamma}^t \tag{3.4b}$$

$$\boldsymbol{u} = \boldsymbol{g} \text{ on } \Gamma^g \tag{3.4c}$$

$$\llbracket \boldsymbol{\sigma} \rrbracket \cdot \boldsymbol{n} = \boldsymbol{0} \text{ across } S \tag{3.4d}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, \boldsymbol{b} the body force vector, $\boldsymbol{\nu}$ the outward unit normal vector to Γ^t , \boldsymbol{t}^{σ} the traction on Γ^t , \boldsymbol{g} the prescribed displacement on Γ^g , and $[\boldsymbol{\sigma}]$ is the jump in stress across S.

200 3.2. Onset of localization: bifurcation analysis

In the material failure mechanics, there exist different approaches to investigate the onset of localized deformation in terms of macrocracks and/or deformation bands. Among them we can point out the local path-independent

criterion (Haghighat and Pietruszczak (2015)), bifurcation analysis (Tjioe 204 and Borja (2016); Borja et al. (2013); Regueiro and Foster (2011)), criti-205 cal plane framework (Pietruszczak and Mroz (2001)). For inelastic mate-206 rials such as those considered here, linear elastic fracture theory cannot be 207 used. Nonlinear theories, such as the J-Integral, have been applied within the 208 eXtended Finite Element Method (e.g Duflot (2007); Mohammadi (2008)). 209 This theory, however, requires path integration through several elements and 210 adapting the integration points to calculate the integral, and may not be path 211 independent for complex plasticity models that may experience unloading. 212 Bifurcation theory, in contrast, depends solely on the local tangent modulus 213 in the small strain case, and hence is often used in conjunction with plasticity 214 and damage models. 215

In this section, the localization condition is derived in terms of bifurcation 216 analysis in conjunction with the cap plasticity model proposed earlier in Sec-217 tion 2. This theory is originated at first by the work of Hill (1962) to explore 218 the onset of inelastic behavior in solids using the physics of wave propagation 210 through the matter. Later on Rudnicki and Rice (1975) adopted this work 220 to develop mathematical framework for detecting shear band localization in 221 solids. It has been shown (Regueiro and Foster (2011); Rice and Rudnicki 222 (1980)) that continuous bifurcation precedes discontinuous case. For contin-223 uous bifurcation, the plastic loading appears outside and within the discon-224 tinuity band at the instant of localization. Thus for strong discontinuities 225

²²⁶ the plastic consistency parameter reads:

$$\dot{\gamma} = \dot{\bar{\gamma}} + \dot{\gamma}_{\delta} \delta_S \tag{3.5}$$

Similarly, in order for the stress-like internal state variables (ISVs), including the backstress α and the isotropic hardening parameter κ , to be bounded (and the plastic dissipation to be well-defined, the hardening moduli c^{α} and c^{κ} have distributional forms (Simo et al. (1993); Regueiro and Foster (2011))

$$(c^{\alpha})^{-1} = (\bar{c}^{\alpha})^{-1} + (c^{\alpha}_{\delta})^{-1} \delta_{S}$$
$$(c^{\alpha})^{-1} \dot{\alpha} = \dot{\gamma} G^{\alpha} \operatorname{dev} \left(\frac{\partial g}{\partial \sigma}\right)$$
$$\dot{\alpha} = \bar{c}^{\alpha} G^{\alpha} \dot{\gamma} \operatorname{dev} \left(\frac{\partial g}{\partial \sigma}\right) = \bar{\boldsymbol{h}}^{\alpha} \dot{\gamma}$$
$$\dot{\alpha} = c^{\alpha}_{\delta} G^{\alpha} \dot{\gamma}_{\delta} \operatorname{dev} \left(\frac{\partial g}{\partial \sigma}\right) = \boldsymbol{h}^{\alpha}_{\delta} \dot{\gamma}_{\delta}$$
(3.6)

$$(c^{\kappa})^{-1} = (\bar{c}^{\kappa})^{-1} + (c^{\kappa}_{\delta})^{-1} \delta_{S}$$
$$(c^{\kappa})^{-1} \dot{\kappa} = \dot{\gamma} G^{\kappa} tr\left(\frac{\partial g}{\partial \sigma}\right)$$
$$\dot{\kappa} = \bar{c}^{\kappa} G^{\kappa} \dot{\gamma} tr\left(\frac{\partial g}{\partial \sigma}\right) = \bar{h}^{\kappa} \dot{\bar{\gamma}}$$
$$\dot{\kappa} = c^{\kappa}_{\delta} G^{\kappa} \dot{\gamma}_{\delta} tr\left(\frac{\partial g}{\partial \sigma}\right) = h^{\kappa}_{\delta} \dot{\gamma}_{\delta}$$
(3.7)

Substitution of Eqs.(3.5), (3.6) and (3.7) in consistency condition, and solving
for both regular and singular parts of the consistency condition gives

$$\dot{\bar{\gamma}} = \frac{1}{\bar{\chi}} \frac{\partial f}{\partial \sigma} : \mathbf{C}^{e} : \dot{\boldsymbol{\epsilon}}^{0}$$

$$\bar{\chi} = \frac{\partial f}{\partial \sigma} : \mathbf{C}^{e} : \frac{\partial g}{\partial \sigma} - \frac{\partial f}{\partial \alpha} : \bar{\boldsymbol{h}}^{\alpha} - \frac{\partial f}{\partial \kappa} \bar{\boldsymbol{h}}^{\kappa}$$

$$\dot{\gamma}_{\delta} = \frac{\frac{\partial f}{\partial \sigma} : \mathbf{C}^{e} : \operatorname{sym}(\llbracket \dot{\boldsymbol{u}} \rrbracket \otimes \boldsymbol{n})}{\frac{\partial f}{\partial \sigma} : \mathbf{C}^{e} : \frac{\partial g}{\partial \sigma}}$$
(3.8a)
$$(3.8b)$$

In addition, we can write the stress rate on the discontinuity surface $\dot{\sigma}^1$ and outside that surface $\dot{\sigma}^0$ as below

$$\dot{\boldsymbol{\sigma}}^{1} = \underbrace{\left(\boldsymbol{C}^{e} - \frac{1}{\chi}\boldsymbol{C}^{e} : \frac{\partial g}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial f}{\partial \boldsymbol{\sigma}} : \boldsymbol{C}^{e}\right)}_{\bar{\boldsymbol{C}}^{ep}} : \dot{\boldsymbol{\epsilon}}^{0} + \tag{3.9a}$$

$$\underbrace{\left(\boldsymbol{C}^{ep} - \frac{\boldsymbol{C}^{e} : \frac{\partial g}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial f}{\partial \boldsymbol{\sigma}} : \boldsymbol{C}^{e}}{\frac{\partial f}{\partial \boldsymbol{\sigma}} : \boldsymbol{C}^{e} : \frac{\partial g}{\partial \boldsymbol{\sigma}}}\right)}_{\bar{\boldsymbol{C}}^{ep}} : \operatorname{sym}\left(\llbracket \dot{\boldsymbol{u}} \rrbracket \otimes \boldsymbol{n}\right) \delta_{S}$$

$$\dot{\boldsymbol{\sigma}}^0 = \bar{\boldsymbol{C}}^{ep} : \dot{\boldsymbol{\epsilon}}^0 \tag{3.9b}$$

where $\tilde{\boldsymbol{C}}^{ep}$ is recognized as the elastic-perfectly plastic tangent modulus.

On the basis of Eq. (3.4d), imposing the traction continuity across the discontinuity surface $(\dot{\sigma}^1 \cdot \boldsymbol{n} = \dot{\sigma}^0 \cdot \boldsymbol{n})$ constitutes the classical condition on

the localization tensor \tilde{A} already identified in Regueiro and Foster (2011).

$$\underbrace{(\underline{\boldsymbol{n}} \cdot \tilde{\boldsymbol{C}}^{ep} \cdot \underline{\boldsymbol{n}})}_{\tilde{\boldsymbol{A}}} \llbracket \dot{\boldsymbol{u}} \rrbracket \, \delta_{S} = 0$$

$$\Rightarrow \det \tilde{\boldsymbol{A}} = 0 \text{ for } \llbracket \dot{\boldsymbol{u}} \rrbracket \neq \underline{0} \qquad (3.10)$$

in which n indicates the most critical orientation of the discontinuity surface in the localized element. The above equation states that a nontrivial solution for the traction continuity condition is, of course, possible only when \tilde{A} is singular.

For discontinuous bifurcation, we assume that the plastic loading is localized to the discontinuity band ($x \in S$), whereas the material points immediately adjacent to the band transfer into an elastic unloading state. As a result, the consistency parameter takes the form of

$$\dot{\gamma} = \dot{\gamma}_{\delta} \delta_S \tag{3.11}$$

Similarly, the hardening moduli would bifurcate in order to have well-definedplastic dissipation.

$$(c^{\alpha})^{-1} = (c^{\alpha}_{\delta})^{-1} \delta_S$$
 and $(c^{\kappa})^{-1} = (c^{\kappa}_{\delta})^{-1} \delta_S$ (3.12)

Furthermore, by imposing traction continuity requirement, again we can arrive at the localization condition manifested in Eq.(3.10). Following the Foster et al. (2007), we use a numerical algorithm to solve det $\tilde{A} = 0$ for the band normal n and then $\tilde{A} \llbracket \dot{u} \rrbracket = 0$ for the deformation directions at the inception of localization.

250 3.3. Evolution of the displacement jump: post-localization model

In this section, a post-localization model is introduced to describe the softening response of the material after localization detection. In particular, a novel cohesive traction-separation law recently presented in Weed et al. (2015) is utilized to characterize the macro-crack evolution in terms of the displacement jump on the slip surface S. Therefore, similar to the concept of cohesive zone models for quasi-brittle materials (see Camacho and Ortiz (1996); Carol et al. (1997); Sancho et al. (2006); de Borst et al. (2006)), a damage-like function F is proposed in two forms of the tensile and compressive regime as below:

$$F_{\text{tension}} = \underbrace{\sqrt{\left(\tau_s\right)^2 + \left(\alpha_\sigma \left\langle\sigma_n\right\rangle\right)^2}}_{\sigma_{\text{eq}}} - c_{\text{eq}}$$
(3.13a)

$$F_{\text{compression}} = |\tau_s - c_{\text{eq}} \cdot \text{sign}(\zeta_s)| - \langle -\sigma_n \rangle \tan\phi' \qquad (3.13b)$$

where the normal traction σ_n and tangential traction τ_s attribute to the slip surface. The notation $\langle \bullet \rangle$ represents the Macaulay brackets, taking into account the positive portion, α_{σ} is a normal stress weighting factor and ϕ' is the friction angle on the slip surface. In addition, the non-negative parameters σ_{eq} and c_{eq} indicate the equivalent traction and equivalent cohesive strength of the band, respectively. Notably, the term sign (ζ_s) devised in Eq. 3.13b would imply that the cohesion on the slip surface operates as a restoring force, i.e. the force c_{eq} always acts in the opposite direction of the displacement jump (or separation) vector. The initial cohesion c_0 is computed in a manner to be balanced with the bulk stress state at the moment of localization.

In the literature, various softening relations have been proposed for a 261 wide range of materials, such as trapezoidal function for a high-strength-262 low-alloy (HSLA) steel (Scheider and Brocks (2003)); exponential function 263 for a C-300 steel (Ortiz and Pandolfi (1999)); linear softening function for a 264 polycrystalline brittle materials (Espinosa and Zavattieri (2003); Benedetti 265 and Aliabadi (2013)); and linear, bilinear, and exponential softening func-266 tions for concrete (Galvez et al. (2002); Bazant (2002)). Here, however, a 267 linear softening curve is adopted for the sake of simplicity. Furthermore, for 268 rock materials like limestone, a linear model has been found to be adequate 269 (Rinehart et al. (2015)). Therefore as depicted in Fig. 5, for the tensile 270 regime the elliptical damage surface F = 0 shrinks to the origin while c_{eq} 271 decreases linearly toward zero as the equivalent displacement jump increases. 272

$$c_{\rm eq} = c_0 \left(1 - \frac{\zeta_{max}}{\zeta_c} \right) \tag{3.14}$$

where ζ_c denotes to the characteristic slip (or separation) distance, beyond which complete failure occurs in the sense that the crack surface entirely loses its cohesive strength. The scalar ζ_{eq} indicates the equivalent jump magnitude 276 and takes the form of

$$\zeta_{\rm eq} = \sqrt{\zeta_s^2 + (\alpha_\zeta \zeta_n)^2} \tag{3.15}$$

in which the variables ζ_n and ζ_s are normal opening and tangential (in-plane 277 sliding) slip on the localization band. The parameter α_{ζ} is a coefficient weigh-278 ing the relative contribution of the opening and sliding modes in the damage 279 process. Following the spirit of damage mechanics in the unloading/reloading 280 case, we assume c_{eq} unloads elastically to the origin. Likewise, the reload-281 ing path is also considered elastic until the point of maximum equivalent 282 separation ζ_{max} attained up until the current time. Beyond this point the 283 softening process will resume. The slope of the unloading-reloading curve 284 can be thought of as the stiffness of the cohesion force and derived as 285

$$k_c = \frac{c}{\zeta_{max}} = c_0 \left(\frac{1}{\zeta_{max}} - \frac{1}{\zeta_c} \right) \tag{3.16}$$

Subsequently, the equivalent stress on the band can be rewritten as (Weed et al. (2015))

$$\sigma_{\rm eq} = k_c \,\zeta_{\rm eq} \tag{3.17}$$

In a number of previous studies, (for example Borja et al. (2013); Foster et al. (2007); Chen et al. (2011)), only one degree of freedom is incorporated into the model which represents sliding displacement with a jump dilation angle ψ' with respect to the discontinuity surface for non-associated plastic-

ity models. It should be remarked that the single sliding degree of freedom 292 may cause spurious hardening and/or a geometric locking effect during non-293 smooth crack propagation. Particularly, in the mixed mode fracture where 294 crack kinking phenomena are frequently observed, using the one-dimensional 295 separation law could trigger slippage impedance in the deformation band, 296 ultimately resulting in significant convergence problem for numerical imple-297 mentation. The model proposed in this study tackles this issue allowing 298 the crack surfaces to separate in a coupled opening and sliding mode in the 299 tensile regime. 300



Figure 5: Cohesive fracture law: (a) isotropic softening of the damage-like surface $F = \theta$ in traction (σ_n, τ_s) space (b) equivalent traction-separation relationship with corresponding loading-unloading paths. ζ_{max} indicates the maximum attained equivalent separation.

The specific fracture energy G is the amount of external energy required to form a unit surface area of the fully-separated (or damaged) crack. This softening property can be simply computed from the area under the tractionseparation function in Fig. 5b. In view of this fact, we can assign different specific fracture energies to each of the respective failure modes (I and II) by 306 assigning $\alpha_{\sigma}, \alpha_{\zeta} \neq 1$.

$$\alpha_{\sigma}\alpha_{\zeta} = \frac{G_{II}}{G_I} \tag{3.18}$$

³⁰⁷ In this work, we will assume $\alpha_{\sigma} = \alpha_{\zeta}$, hence

$$\alpha_{\sigma} = \alpha_{\zeta} = \left(\frac{G_{II}}{G_I}\right)^{\frac{1}{2}} \tag{3.19}$$

It is worth noting that in the compressive case (i.e., crack closure), the frictional resistance always operates on the crack surface independently of the softening process. Indeed, once the cohesion strength completely degrades $(\zeta_{max} = \zeta_c)$, the cohesive crack surface evolves to a Coulomb friction surface with friction coefficient $\mu = \tan \phi'$. In this work, we consider a static coefficient of friction, though to get more realistic results a variable coefficient, as in Borja and Foster (2007); Foster et al. (2007), can be used.

315 4. Finite element implementation: the AES method

In order to incorporate strong discontinuity analysis into the platform of finite element simulation, the assumed enhanced strain (AES) method based on the Hu-Washizu principle is invoked (Borja (2008); Foster et al. (2007); Simo et al. (1993)). In this approach, the displacement discontinuity is conceptualized as an appropriate incompatible mode and added to the standard FE solutions. Note that the AES method is numerically appealing technique since the enhancements for discontinuities are condensed out locally and hence no additional global degrees of freedom are added to the calculations. In doing so, the standard static condensation algorithm is considered
to confine the enhancement within the element level.

Figure 6 demonstrates the underlying idea behind the finite element implementation. As shown, a constant strain triangle (CST) element is traced by a discontinuity surface S^e . In addition, we postulate a piecewise constant interpolation of the displacement jump, i.e. $[\![\boldsymbol{u}]\!] = \zeta \boldsymbol{m}$.



Figure 6: Enhancing a CST finite element: (a) element breaks into two parts (triangle with bold lines represents the conforming deformation.); Vectors \boldsymbol{n} and \boldsymbol{s} indicate the normal and tangential separations across the S^e , respectively. (b) displacement field with a jump across a slip plane.

³³⁰ The strain rate tensor for infinitesimal deformation is written as

$$\dot{\boldsymbol{\epsilon}} = \nabla^{s} \dot{\boldsymbol{u}} = \underbrace{\nabla^{s} \dot{\boldsymbol{u}}}_{conforming} + \underbrace{\left(-\begin{bmatrix} \dot{\boldsymbol{u}} \end{bmatrix} \otimes \nabla f^{h}\right)^{s} + \left(\begin{bmatrix} \dot{\boldsymbol{u}} \end{bmatrix} \otimes \boldsymbol{n}\right)^{s} \delta_{S}}_{enhanced}$$
(4.1)

³³¹ which can be regularized in a form of

$$\dot{\boldsymbol{\epsilon}} = \nabla^{s} \dot{\boldsymbol{u}} = \underbrace{\nabla^{s} \dot{\boldsymbol{u}} + \left(-\begin{bmatrix} \dot{\boldsymbol{u}} \end{bmatrix} \otimes \nabla f^{h}\right)^{s}}_{\dot{\boldsymbol{\epsilon}}^{reg}} + \underbrace{\left(\begin{bmatrix} \dot{\boldsymbol{u}} \end{bmatrix} \otimes \boldsymbol{n}\right)^{s} \delta_{S}}_{singular}$$
(4.2)

The function $f^h(\boldsymbol{x})$ is a smooth blending function for localized elements that may be conveniently defined as the sum of the shape functions attributed to the active nodes.

$$f^{h} = \sum_{A=1}^{n_{en}} N_{A} H_{S} \left(\boldsymbol{x}_{A} \right)$$

$$\tag{4.3}$$

where n_{en} is the number of nodes for a localized element, and N_A are the 335 standard finite element shape functions. Using such a kinematic description 336 affords the formulation the ability to allow the essential boundary conditions, 337 Γ^{g} in Figure 4, to be applied exclusively on the conforming displacement term 338 $\tilde{\boldsymbol{u}}(\boldsymbol{x},t)$. As a result, the nodal displacements calculated at the global level 339 can be realized as the final displacements. Eventually, the finite element 340 stress for localized elements can be obtained from the regular part of the 341 strain $\dot{\boldsymbol{\epsilon}}^{reg}$. The relevant mathematical background is discussed in Borja and 342 Regueiro (2001). Thus, for elastic unloading we have 343

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{C}^e : \dot{\boldsymbol{\epsilon}}^{reg} \tag{4.4}$$

For further details of the AES method, including its variational and matrix formulation, the reader is referred to Borja (2008) and the references 346 therein.

347 5. Numerical implementation

Numerical integration of the constitutive models plays a pivotal role in successfully modeling boundary value problems in engineering. Herein, a well established integration technique called the implicit return mapping algorithm is invoked. This algorithm affords first-order accuracy while satisfying the conditions for unconditional stability.

353 5.1. Cap plasticity model

To solve the non-linear material model proposed in Section 2, we employ the well-known Newton-Raphson (N-R) iterative method. This method basically constructs the residual vector \boldsymbol{R} as a function of the unknown variables \boldsymbol{X} as below:

$$\boldsymbol{R}(\boldsymbol{X}) = \begin{cases} \Delta \boldsymbol{\sigma} + \Delta \gamma [\boldsymbol{C}^{e}] \cdot \left(\frac{\partial g}{\partial \boldsymbol{\sigma}}\right) - \boldsymbol{C}^{e} : \Delta \boldsymbol{\epsilon} \\ \Delta \boldsymbol{\alpha} - \Delta \gamma \boldsymbol{h}^{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) \\ \Delta \boldsymbol{\kappa} - \Delta \gamma \boldsymbol{h}^{\boldsymbol{\kappa}}(\boldsymbol{\kappa}) \\ f(\boldsymbol{\sigma}, \boldsymbol{\alpha}, \boldsymbol{\kappa}) \end{cases} \quad \text{in which } \boldsymbol{X} = \begin{cases} \boldsymbol{\sigma} \\ \boldsymbol{\alpha} \\ \boldsymbol{\kappa} \\ \Delta \gamma \end{cases}$$
(5.1)

where $[\mathbf{C}^e]$ is the linear elastic stiffness matrix in the Voigt form and $\Delta \gamma$ is the discrete consistency parameter. Here $\boldsymbol{\sigma}$ and $\boldsymbol{\alpha}$ are the Voigt form of the Cauchy stress and backstress tensors, respectively. The implicit stressintegration algorithm is summarized in the Appendix Box 1.

362 5.2. Post-localization model

Regarding the nonlinear formulation proposed for the combined openingsliding fracture evolution Eq. 3.13a, we use the standard N-R algorithm to solve for displacement jump $\boldsymbol{\zeta} = (\zeta_n, \zeta_s)$ on the band. As a result, the residual vectors can be defined based on traction balances on the band taking the form of:

$$\Phi_1 = \langle \sigma_n \rangle - k_c \zeta_n = 0 \tag{5.2a}$$

$$\Phi_2 = |\tau_s - k_c \zeta_s| - \langle -\sigma_n \rangle \tan \phi' = 0$$
(5.2b)

It is worth it to mention that in the tensile regime, the residual Φ_2 can be reattained as $\tau_s - k_c \zeta_s = 0$. On the other hand, in the compression case, we can solve only the second residual Φ_2 with no need for any iterative methods. Implicit integration of slip values in terms of whether the slip band is newly detected or if the displacement jump evolution has already been activated on the band is presented in the Appendix (Box 2 and Box 3, respectively).

³⁶⁹ 6. Numerical efficiency and robustness

370 6.1. Cap plasticity model

Particular mathematical treatments can be exploited to improve the ef-371 ficiency and robustness of the integration procedure. The first remedy is 372 reducing the number of unknowns in the system of nonlinear equations as 373 the cap plasticity model can be as large as 13 (6 for stress components, 5 for 374 kinematic hardening, 1 for isotropic hardening and 1 for consistency param-375 eter). This number can be reduced to 7 using the spectral decomposition 376 method and sometimes to 6 when the priori shear/cap surface determination 377 technique is applied as well. 378

In addition to this, the consistent tangent modulus $\boldsymbol{C}_{n+1}^{alg} = \partial \boldsymbol{\sigma}_{n+1} / \partial \boldsymbol{\epsilon}_{n+1}$ 379 is computed in order to gain the quadratic rate of convergence within the 380 framework of implicit integration algorithm. To this end, another remedy 381 which can be applied is recasting the residual vectors with a uniform dimen-382 sionality. This feature could enhance the robustness and tractability of the 383 Newton-Raphson procedure as improves the conditioning of the local tangent 384 matrix $D\mathbf{R}/D\mathbf{X}$ and also reduces the number of iterations required to reach 385 the convergent solutions for X. For further elaboration of these algorithms 386 the interested reader is referred to Motamedi and Foster (2015) and Foster 387 et al. (2005). 388

389 6.2. Post-localization model

390 6.2.1. Spurious solutions

Since there is no guarantee whether a trial guess for the state of the 391 band (being in tension or compression) stays valid during the integration 392 procedure, the N-R iteration may converge to a spurious solution for slip 393 value(s). To overcome this drawback, once a change in the sign of the normal 394 traction is detected, the slip on the band should be instead calculated using 395 the appropriate formulation with regard to the new state of the band. Owing 396 to this, a standard linear interpolation is utilized to find a new slip value as 397 the starting point of the subsequent N-R. 398

$$\zeta_s = \zeta_s^i - \sigma_n^i \cdot \left(\frac{\zeta_s^f - \zeta_s^i}{\sigma_n^f - \sigma_n^i}\right) \tag{6.1}$$

where (σ_n^i, ζ_s^i) are the initial normal traction and slip values at the beginning of the N-R iteration, (σ_n^f, ζ_s^f) are the spurious converged values and ζ_s is the interpolated shear slip value corresponding to the critical point $(\sigma_n, \zeta_n) =$ (0, 0) in which the sign of the normal traction changes.

403 6.2.2. Impl-Ex integration scheme

In the finite element simulation of materials undergoing strain softening behavior, even if the nonlinear problem is mathematically well posed and features a unique solution, it is well known that the classical implicit approach may suffer from a lack of robustness during a given iterative procedure. As discussed in detail by Oliver et al. (2006a), if material failure propagates through the solids, the tangent constitutive operator C_{n+1}^{alg} progressively loses its positive definite character which is eventually accompanied by the loss of positive definiteness of the global stiffness matrix.

In order to ameliorate the shortcomings of the fully implicit schemes, we apply an implicit/explicit (Impl-Ex) integration technique adopted from Oliver et al. (2006a). Using this semi-implicit algorithm to seek solution at time step t_{n+1} , the slip values $\boldsymbol{\zeta}$ are explicitly approximated based on their implicitly updated values from prior time steps t_n and t_{n-1} .

$$\tilde{\boldsymbol{\zeta}}_{n+1} = \boldsymbol{\zeta}_n + \frac{\Delta t_{n+1}}{\Delta t_n} \left(\boldsymbol{\zeta}_n - \boldsymbol{\zeta}_{n-1} \right)$$
(6.2)

417 The semi-implicit stress is then calculated

$$\tilde{\boldsymbol{\sigma}}_{n+1} = \boldsymbol{\sigma}_n + \boldsymbol{c}^e : \Delta \boldsymbol{\varepsilon}_{n+1}^{\text{conf}} - \boldsymbol{c}^e : \left(\tilde{\boldsymbol{\zeta}}_{n+1} \otimes \nabla f^h \right)^s$$
(6.3)

since $\hat{\zeta}_{n+1}$ is postulated as a predetermined vector, we can easily derive the effective algorithmic operator C_{n+1}^{eff} as below

$$\boldsymbol{C}_{n+1}^{\text{eff}} = \frac{\partial \tilde{\boldsymbol{\sigma}}_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = \boldsymbol{C}^{e}$$
(6.4)

Hence, for linear elasticity, the tangent modulus is constant. The modification of taking the entire slip vector, rather than the magnitude as used in
Oliver et al. (2006a) was proposed in Weed et al. (2015). This approach, at
minor cost of accuracy, improved the efficiency of the simulation by creating



Figure 7: Flowchart for the numerical integration algorithm within a FE code: (a)Implicit scheme, (b)Impl-Ex scheme.

a linear solution in this part. It should be commented that unconditional stability is lost in the system. At the end of the time step, once the convergent solution of the global displacements is obtained, the stress σ and slip values ζ will be implicitly updated to be used as a reference point for the next time step. A flowchart given in Fig. 7 schematically illustrates the difference between the new semi-implicit scheme and the conventional fully implicit algorithm.

431 7. Numerical benchmark problem:

The cracked Brazilian disc (CBD) test is one of the most acknowledged 432 methods in evaluating mixed-mode fracture behavior of brittle geomaterials. 433 Among the numerous experimental tests that have been conducted in this 434 specimen for different rock materials, we can mention to Keochang gran-435 ite (Chang et al. (2002)), Yeosan marble (Chang et al. (2002)), Saudi Ara-436 bian limestone (Al-Shayea (2005)), Guiting limestone (Aliha et al. (2010)), 437 Dionysos marble (Kourkoulis et al. (2012)), and Neyriz marble (Ayatollahi 438 and Akbardoost (2014)). In this study, the material properties listed in Ta-439 ble 1 were fit to Salem limestone rock by Fossum and Brannon (2004) and 440 frequently reported in Regueiro and Foster (2011), Sun et al. (2013) and 441 Motamedi and Foster (2015). For the specific fracture energy ratio G_{II}/G_I , 442 varied values are calculated experimentally dependent on the specific mate-443 rial of the interest and the fracture test chosen. In this paper, we use the 444 empirical value of $G_{II}/G_I = 4.8$. This value is given in Al-Shayea (2005) 445 for a Saudi Arabian limestone rock tested under the ambient condition us-446 ing CBD configuration. For the characteristic slip distance ζ_c , the value 0.4 447 (mm) is assumed (Borja and Foster (2007)). 448

The generic configuration of the test is illustrated in Fig.(8) and the same as one utilized in the experimental test by Al-Shayea (2005). The circular disk contains a radius R=49mm as well as the crack length ratio a/R = 0.3. The angle β stands for orientation of the crack with respect to the loading direction \boldsymbol{u} .

Table 1: Material parameters for Salem limestone rock used in the CBD test

Parameter	Value		
Young's Modulus (E)	22547 (MPa)		
Poisson's Ratio (ν)	0.2524 (dimensionless)		
isotropic tensile strength (T)	5 (MPa)		
tension cap parameter (I_1^T)	0.0 (MPa)		
compression cap parameter (κ_0)	-8.05 (MPa)		
shear yield surface parameter (A)	689.2 (MPa)		
shear yield surface parameter (B)	3.94e-4 (1/MPa)		
shear yield surface parameter (L)	1.0e-4 (1/MPa)		
shear yield surface parameter (C)	675.2 (MPa)		
shear yield surface parameter (θ, ϕ)	$0.0 ({\rm rad})$		
aspect ratios (R, Q)	28.0 (dimensionless)		
isotropic hardening parameter (W)	0.08 (dimensionless)		
isotropic hardening parameter (D_1)	1.47e-3 (1/MPa)		
isotropic hardening parameter (D_2)	$0.0 \; (1/MPa^2)$		
kinematic hardening parameter (c^{α})	1e5 (MPa)		
kinematic hardening parameter (N)	6.0 (MPa)		
stress triaxiality parameter (ψ)	0.8 (dimensionless)		
localized friction angle (ϕ')	$40^{\circ}(\text{degree})$		
characteristic slip distance (ζ_c)	$0.4 \;({\rm mm})$		
specific fracture energy ratio (G_{II}/G_I)	4.8 (dimensionless)		



Figure 8: Geometry and loading conditions of CBD specimen subjected to mixed mode $\rm I/II$ loading.

The displacement-controlled loading test is replicated via applying the 454 vertical displacement on the three nodes of top surface of the disk. The 455 three nodes at the bottom surface are fixed in the vertical direction. In order 456 to maintain the global stability of the example, the two nodes located at the 457 crest and trough of the disk are restricted from lateral movement as well. 458 To investigate the effect of mode mixity on crack growth path and failure 459 pattern, the example is performed with three different crack inclination angles 460 $(\beta = 15^{\circ}, 30^{\circ}, \text{ and } 55^{\circ})$. In view of the fact that all aforementioned CBD 461 tests captured a clear, continuous fracture surface for rock specimens, we 462 check the localization condition only for tip elements. Hence, the new crack 463 surface will be traced from the crack tip at one edge of the tip element to the 464 opposite edge with the orientation obtained from discontinuous bifurcation 465 analysis described in Section 3.2. This algorithm is visualized schematically 466 in Figure 9. The detection algorithm is only performed at the end of each 467 time step for simplicity. While this introduces some error, it has been shown 468 that the error disappears as the time step is refined Parvaneh and Foster 469 (2016).470

To perform the FE simulation, a mesh with 512 CST elements is employed, Figure 10. Deformations are assumed to be infinitesimal. Several theoretical and experimental studies conducted in the past on rock samples with various thicknesses suggest that the specimen thickness has negligible effect on fracture behavior of rock materials (see for example Whittaker et al. (1992) and Khan and Al-Shayea (2000)). As a result, this example is ana-



Figure 9: Strategy for tracing the crack propagation path.

477 lyzed under plane strain condition.

The initial central cracks are introduced in the FE model as a fully damaged part of the specimen using the specific embedded discontinuity surfaces inside the elements as graphically shown in Figure 10. This interface includes zero initial cohesive strength and localized friction angle so that the pre-cracked elements immediately fail when loaded in tension, shear or any of their combinations. These elements can, however, still endure compressive loads.

The paths of crack propagation for three inclination angles are depicted in Figure 10. This plot indicates that the fracture propagation initiates from both ends of the pre-existing cracks, and kinks into a new direction. Subsequently the crack growth continues along a curved path toward the direction of loading. This numerical prediction is quite similar to experimental observations in several laboratory studies, see for example Al-Shayea (2005), ⁴⁹¹ Aliha et al. (2010) and Haeri et al. (2014), among others.

The reaction force-versus-downward displacement response is presented 492 in Figure 11. The numerical procedure adequately converges until the end 493 of the curves, to practically null load \boldsymbol{u} . For inclination angles β equal to 494 30 and 55 degrees, there is a convergence issue as the crack approaches the 495 displacement boundaries. As pointed out by Chen et al. (2011) in the AES 496 method, discontinuities which propagate into essential boundary conditions 497 will have difficulty converging. In order to avoid this, they suggest rotating 498 the discontinuity surface slightly so that there is at least one element between 499 the localized elements and the elements which have the assigned boundary 500 conditions. But for $\beta = 10$ degrees, the entire simulation finishes successfully 501 and a complete softening curve is obtained. Furthermore, the end of the 502 softening curve displays a slight rise in the residual force, which is most 503 likely due to friction effects on the discontinuity surface. There is a noticeable 504 discrepancy between $\beta = 30$ degrees and the two other inclinations angles 505 (10 and 55 degrees) with regard to the maximum reaction force. From the 506 simulation results, the 30 degree angle produces a stress state, within the 507 tip elements, which is more critical for bifurcation analysis than the other 508 two angles. Aliha et al. (2010) carried out different CBD tests for Guiting 509 limestone to investigate the geometry and size effects on fracture trajectory 510 under mixed mode loading. They show that the $\beta = 27$ degrees produces a 511 minimum fracture load, which is in close accord with our simulation results. 512 According to their analytical calculations, derived based on GMTS criterion, 513

this discrepancy could be attributed to the magnitude and sign of the Tstress.

The crack initiation angle θ' is the angle by which the crack extension 516 deviates from the direction of the initial crack inserted inside the specimen. 517 The values of θ' are derived based on bifurcation analysis for tip localized 518 elements and shown in Table 2. Results are compared with the experimen-519 tal data provided in Al-Shayea (2005). For lower inclination angles, $\beta = 15$ 520 and 30 degrees, numerical results accords well with the experiment. But for 521 $\beta = 55^{\circ}$, there is a gap between the results. The main reason for this differ-522 ence is that the model could not consider the influence of the crack closing 523 which indeed observed in the laboratory tests. However, If the crack initia-524 tion angle is recalculated for the first two tip elements, the θ' approaches to 525 the corresponding experimental value. In other words, numerical simulation 526 adjusts its crack path orientation shortly after the slip evolution proceeds in 527 initial cracks. 528

Table 2: Crack initial angle θ' for CBD test

Inclination angle	$\beta = 15^{\circ}$	$\beta = 30^{\circ}$	$\beta = 55^{\circ}$	
Experimental test (Al-Shayea (2005)) Numerical simulation	$\frac{26}{27^{\circ}}^{\circ}$	${70}^\circ {66}^\circ$	$81^{\circ} \\ 58^{\circ} (77.5^{\circ})^{*}$	
* The average crack initial angle for the first two tip elements				

529

In the study of the fracture behavior of the disk specimen, additional insights
can be gained by comparing the kinematics of deformation. Accordingly, the

deformed meshes generated by the AES solution are displayed in Figures 532 12-14. When the disc is loaded under diametral compression, for lower in-533 clination angles $\beta = 10^{\circ}$ and 30° the two faces of the initial coplanar crack 534 simultaneously open and slide relative to each other. For inclination an-535 gle $\beta = 55^{\circ}$, by contrast, the results demonstrated in-plane sliding of the 536 central crack faces. This numerical observation compares with experimen-537 tal data reported by Al-Shayea (2005) in which a crack extension et er was 538 attached to the pre-existing cracks with a perpendicular position to its ori-539 entation. As illustrated by the author, for crack angles of $\beta \leq 45^{\circ}$, the 540 sensor recorded positive values. This observation validates the presence of 541 crack opening deformation at the crack mouth. Conversely, by increasing the 542 crack inclination, the crack closure becomes more pronounced which would 543 be characterized in our model as a pure shear sliding mode. While there is 544 some difference between the saw cut of finite width in the experiment and 545 the crack modeled here, the model is more typical of the type of flaws seen 546 in real geosystems. 547

548



Figure 10: Crack propagation path simulation for CBD specimen with different inclination angle (β =10, 30 and 55). Initial cracks are represented by the dash thick lines through the finite element mesh.



Figure 11: Load-displacement plots for CBD specimen with different inclination angle (β =10, 30 and 55).



(a) Horizontal displacement contour (b) Vertical displacement contour Figure 12: Deformed mesh with enhanced solution for inclination angle (β =10).



(a) Horizontal displacement contour (b) Vertical displacement contour Figure 13: Deformed mesh with enhanced solution for inclination angle (β =30).



(a) Horizontal displacement contour
 (b) Vertical displacement contour
 Figure 14: Deformed mesh with enhanced solution for inclination angle (β=55).

549 8. Conclusion

In this paper, a finite element simulation of a mixed-mode fracture propagation for CBD is created. Localized failure is detected by a loss of ellipticity condition, and subsequent post-localization softening is modeled in the framework of an enhanced strain finite element schema. These elements include additional internal degrees of freedom which track both opening and shear displacement on a critically orientated surface determined by bifurcation theory.

⁵⁵⁷ Due to the fact that the accuracy of bifurcation prediction is fundamen-⁵⁵⁸ tally dependent on the constitutive model used in the analysis, a three-⁵⁵⁹ invariant cap plasticity model based on a non-associated flow rule and com-⁵⁶⁰ bined isotropic/kinematic hardening is adopted. The newly added tension ⁵⁶¹ cap to the constitutive model enables us to investigate the inception of dila-⁵⁶² tion bands in addition to shear bands.

To simulate the CBD specimen test, an initial crack is introduced into 563 the model by inserting frictionless interfaces within pre-cracked elements. 564 In addition, assigning a negligible initial cohesion for those cracks leads to 565 the immediate appearance of localized deformations in a form of combined 566 shear/opening fracture. Nevertheless, those pre-localized elements still carry 567 compressive loads as crack closure occurs. The plane strain simulation of the 568 CBD specimen shows good agreement with experimental results contained 569 in the referenced literature. Specifically, the simulation accurately captures 570 the kinking nature of the crack and the overall crack path orientation. 571

For future work, in order to more precisely replicate load transfer, we consider implementing a contact mechanics formulation to model the interface between the boundary constraints (loading platens in the experiments) and the CBD specimen.

576

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579

Appendix

Here, implicit integration algorithms are provided, demonstrating how stress state and displacement jump values are calculated for cap plasticity model and post-localization model, respectively. Box 1: implicit stress-point algorithm for cap plasticity model.

Step 1: Compute trial state variables: $\boldsymbol{\sigma}_{n+1}^{tr} = \boldsymbol{\sigma}_n + \boldsymbol{c}^e : \Delta \boldsymbol{\epsilon}_{n+1}, \quad \boldsymbol{\alpha}_{n+1}^{tr} = \boldsymbol{\alpha}_n, \\ \kappa_{n+1}^{tr} = \kappa_n.$

Step 2: Check the yielding condition: $f_{n+1}^{tr} > 0$?

If no, set $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{tr}$, $\boldsymbol{\alpha}_{n+1} = \boldsymbol{\alpha}_n$, $\kappa_{n+1} = \kappa_n$ and exit. If yes, Go to step 3

Step 3: Apply particular mathematical treatments to reduce the number of unknowns and hence improve the computational efficiency (see Section 6.1):

Step 4: Initialize $X_0 = 0$ and use N-R scheme to solve for converged solution:

$$\begin{split} \delta \boldsymbol{X}^{(k+1)} &= [D\boldsymbol{R}/D\boldsymbol{X}]^{-1}\boldsymbol{R}(\boldsymbol{X}^k) \\ \boldsymbol{X}^{(k+1)} &= \boldsymbol{X}^{(k)} + \delta \boldsymbol{X}^{(k+1)} \\ \text{Until } ||\boldsymbol{R}(\boldsymbol{X})||/||\boldsymbol{R}(\boldsymbol{X}_0)|| < \text{tol}_{\boldsymbol{X}} \\ \text{where } k+1 \text{ refers to the current iteration.} \end{split}$$

Step 5: Update state variables σ_{n+1} , α_{n+1} , κ_{n+1} and consistency parameter γ_{n+1} then exit.

Box 2: Implicit algorithm for a newly localized element.

 $\begin{array}{lll} Step \ 1: & \text{Compute trial state variables:} & \boldsymbol{\sigma}_{n+1}^{tr} &= \boldsymbol{\sigma}_n + \boldsymbol{c}^e &: \ \Delta \boldsymbol{\epsilon}^{reg}, \\ \boldsymbol{\sigma}_{nn+1}^{tr} &= \boldsymbol{\sigma}_{n+1}^{tr} : (\boldsymbol{n} \otimes \boldsymbol{n}) \text{ and } \boldsymbol{\tau}_{sn+1}^{tr} = \boldsymbol{\sigma}_{n+1}^{tr} : (\boldsymbol{s} \otimes \boldsymbol{n}). \end{array}$ $Step \ 2: & \text{Check for yielding on the band:} F_{n+1}^{tr} > 0?$ $\text{If no, band is inactive. Set } \boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{tr} \text{ and } \boldsymbol{\zeta}_{n+1} = \boldsymbol{0} \text{ then exit.}$ If yes, band is active. Go to Step 3. $Step \ 3: & \text{Solve for slip values } \boldsymbol{\zeta}_{n+1} = (\boldsymbol{\zeta}_n, \boldsymbol{\zeta}_s)_{n+1} \text{ on the band:}$ $\text{If } \boldsymbol{\sigma}_n^{tr} > 0 \text{ (tension), If } \boldsymbol{\zeta} = \boldsymbol{0} \text{ then initialize } \boldsymbol{\zeta}_0 = tol \left[\boldsymbol{\sigma}_n, \boldsymbol{\tau}_s\right]_n^T \text{ and use}$ N-R scheme to solve for converged solution: $\delta \boldsymbol{\zeta}_{(k+1)}^{(k+1)} = \left[D \boldsymbol{\Phi}/D \boldsymbol{\zeta}\right]^{-1} \boldsymbol{\Phi}(\boldsymbol{\zeta}^k)$ $\boldsymbol{\zeta}_{(k+1)}^{(k+1)} = \boldsymbol{\zeta}^{(k)} + \delta \boldsymbol{\zeta}^{(k+1)}$ $\text{Until } ||\boldsymbol{\Phi}(\boldsymbol{\zeta})||/||\boldsymbol{\Phi}(\boldsymbol{\zeta}_0)|| < \text{tol} \boldsymbol{\zeta}$ where k + 1 refers to the current iteration. $Step \ 3.1: \text{ Check to avoid spurious solution (see Section 6.2.1).}$ $\text{Else } \boldsymbol{\sigma}_n^{tr} < 0 \text{ (crack closure) then solve for } \boldsymbol{\zeta}_s \text{ using 5.2b.}$

Step 3.2: Check to avoid spurious solution (see Section 6.2.1).

Step 4: Update $\boldsymbol{\zeta}_{n+1}$, $k_{c,n+1}$, and $\boldsymbol{\sigma}_{n+1}$ then exit.

Box 3: Slip algorithm for an element which has pre-existing slip on the band.

Step 1: Compute trial state variables: $\boldsymbol{\sigma}_{n+1}^{tr} = \boldsymbol{\sigma}_n + \boldsymbol{c}^e$: $\Delta \boldsymbol{\epsilon}^{reg}$, $\sigma_{n+1}^{tr} = \boldsymbol{\sigma}_{n+1}^{tr} : (\boldsymbol{n} \otimes \boldsymbol{n})$ and $\tau_{sn+1}^{tr} = \boldsymbol{\sigma}_{n+1}^{tr} : (\boldsymbol{s} \otimes \boldsymbol{n})$.

Step 2: Assume elastic unloading/reloading phase on the band, hence hold k_c as a constant. Set $k_{cn+1} = c_0 \left(\frac{1}{\zeta_{max,n}} - \frac{1}{\zeta_c}\right)$ then:

If $\sigma_n^{tr} > 0$ (tension) solve for slip values $\boldsymbol{\zeta}_{n+1} = (\zeta_n, \zeta_s)_{n+1}$ using the balance equations 5.2a and 5.2b.

Else ($\sigma_n^{tr} < 0$, hence compression)

First, check for slip on the band:

If $|\tau_s - k_c \zeta_s| < \langle -\sigma_n \rangle \tan \phi$

No slip on the band due to frictional lock, exit with trial stress.

Else

Solve for ζ_s using: 5.2b.

Step 2.1: After slip value(s) calculated, evaluate elastic unloading/reloading assumption: $\zeta_{eff_{n+1}} < \zeta_{max,n}$?

If yes, update σ_{n+1} and set $\zeta_{max,n+1} = \zeta_{max,n}$ and exit. If no, the band is in the softening phase, set k_c as a decreasing variable and use Box 2 to solve for slip value(s).

Step 3: Update $\boldsymbol{\zeta}_{n+1}$, $k_{c,n+1}$ and $\boldsymbol{\sigma}_{n+1}$ then exit.

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