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6 **Numerical modeling of the opening mode fracturing emanating from deformation**
7 **localization in layered rocks**

8

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21 **Abstract**

22 It is known that rock fracture includes inelastic straining or damage that should localize at a
23 certain loading stage and result in fracture initiation. The details of this process are not clear,
24 and it is frequently omitted in the models by imposing the initial microcracks (seeds) with
25 certain lengths and orientations. Here we investigate 2-D systems of three layers in finite-
26 difference models. The layers subjected to the horizontal extension are separated by cohesive-
27 frictional interfaces and have contrasted properties typical of sedimentary piles. Fractures are
28 initiated in a more brittle central layer in the vicinity of the interfaces with the adjacent layers.
29 It starts with the initially distributed inelastic straining, which then localized into narrow
30 bands. The damage within these bands is strongly accelerated, resulting in complete material
31 failure locally. Short initial fractures corresponding to narrow bands of failed material are
32 normal to the least local stress. They then propagate from the interfaces to the layer center
33 with further extension. We carefully investigate the impact of different regularization
34 procedures, the grid geometry, and structure on all stages of the fracture process and define
35 the optimal conditions that can be applied for fracture modeling in different structural and
36 loading configurations.

37 *Keywords*

38 Strain localization, pure dilation bands, fracture initiation and propagation, elastoplastic
39 modeling, regularization, layered rocks

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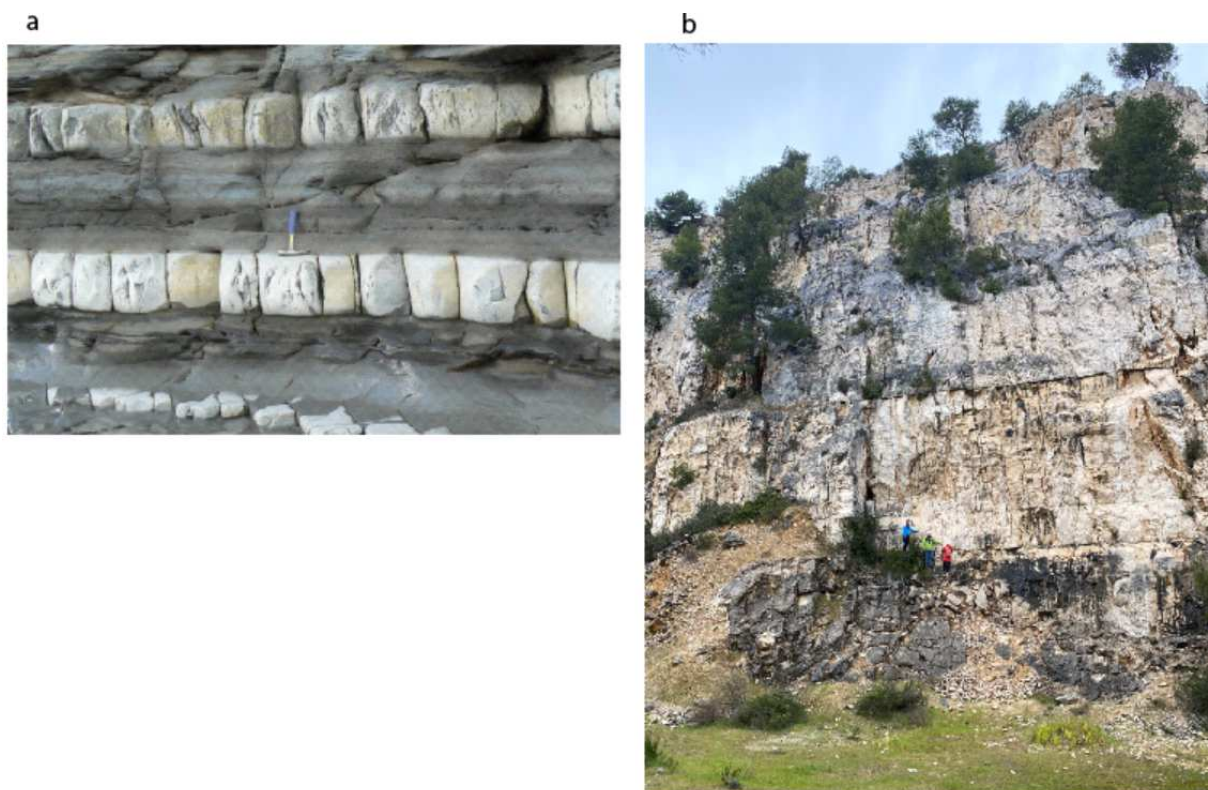
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43 **1 Introduction**

44 The so-called opening mode (mode I) fractures or joints are the most common in the Earth's
45 crust, notably in sedimentary basins, and frequently form regular sets of vertical (bed-normal)
46 parallel, orthogonal, or more complex fracture networks. They strongly impact the mechanical
47 properties and permeability of rock masses and thereby play an essential role in the stability
48 of geological or man-made structures, production of water and hydrocarbons, storage of CO₂,
49 etc. For this reason, joints have been extensively studied for more than a century (e.g., Pollard
50 & Aydin, 1988) with a particular focus on their spatial distribution in relation to the thickness
51 and mechanical proprieties of fractured sedimentary beds, fracture microstructure, and
52 loading conditions (Price, 1966; Hobbs, 1967; Ji et al., 1998; Huang & Angelier, 1989; Narr
53 & Suppe, 1991; Gross, 1993; Engelder et al., 1997; Bai & Pollard, 2000; Gross et al., 1995;
54 Cherepanov, 1997; Tang et al., 2008; Schöpfer et al., 2011; Li et al., 2012; Guo et al., 2017;
55 Ruf et al., 1998; Rustichelli et al., 2013; Cilona et al., 2016; Levi et al., 2019; Bao et al., 2019;
56 Ji et al., 2021).

57 The origin of most joints is believed to be related to the mechanical interaction between
58 sedimentary beds that have contrasted lithological and hence mechanical properties and
59 different thicknesses (Fig. 1). The conceptual scheme typically used to address and predict the
60 formation of these fractures is shown in Fig. 2. A sedimentary pile (Fig. 2a) is subjected to the
61 horizontal extension, which leads to progressive fracturing (sequential fracture infill) of more
62 brittle (competent) layers and non-localized elastic and/or ductile extension of other
63 (incompetent) layers. The setup of numerical models usually includes only three layers, one
64 competent layer sandwiched between two incompetent ones (Fig. 2b).



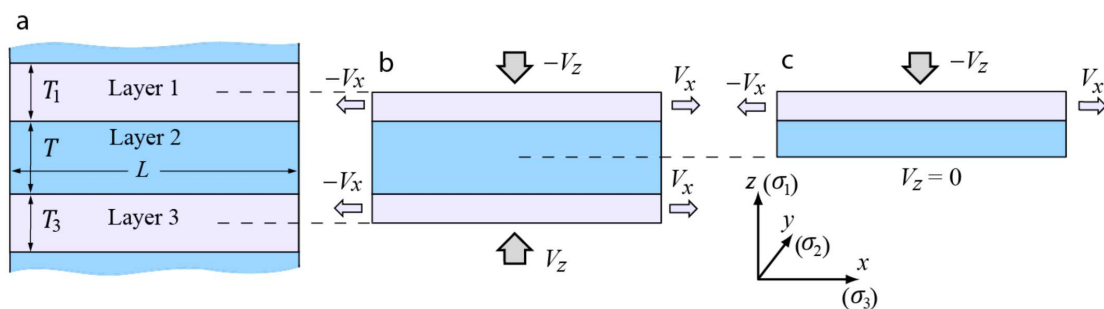
65 **Figure 1.** Field examples of layered and fractured sedimentary rocks. (a) Alternating
 66 incompetent (mudrocks) and fractured competent (limestone) layers in Lilstock Bay,
 67 Somerset, UK (rock hammer for scale) from Schöpfer et al. (2011). (b) Thick densely
 68 fractured Urgonian limestone layers; Cassis, Provence, SE France from Chemenda et al.
 69 (2021).

70

71 In the initial models, the competent layer was elastic, and fracture modeling was based on
 72 Linear Elastic Fracture Mechanics (LEFM) (e.g., Gross et al., 1995; Bai & Pollard, 2000).
 73 Although LEFM is still dominating in the analysis and modeling of natural fracturing (Bai &
 74 Pollard, 2000; Olson et al., 2009; Pollard & Aydin, 1988; Savalli & Engelder, 2005; Segall &
 75 Pollard, 1983; Gross et al., 1995; de Jussineau & Petit 2021), it is evident that inelastic
 76 deformation is involved in and affects this process. The degree of this involvement depends
 77 on the ductility of a fractured material, which in turn depends on its composition, loading
 78 conditions (effective pressure), and lithification stage of sedimentary rocks at fracturing (e.g.,
 79 Paterson & Wong, 2005; Lavenu & Lamarche, 2018; Chemenda, 2019; La Bruna et al.,
 80 2020). The elastic-plastic modeling of fracturing was conducted using different numerical

81 methods (Schöpfer et al., 2011; Tang et al., 2008; Li et al., 2012; Guo et al., 2017; Chemenda
 82 et al., 2021). The layers in these models were either totally coupled or separated by frictional
 83 and/or cohesive interfaces.

84 A linear relation between the thickness T of the fractured layer and the fracture spacing S has
 85 resulted from most modeling studies. The geological data confirm such a relational for $T =$
 86 $T_0 \sim < 1$ m (Engelder et al., 1997; Gross, 1993; Huang & Angelier, 1989; Ji et al., 1998; Narr
 87 & Suppe, 1991; Ruf et al., 1998; Rustichelli et al., 2013; Cilona et al., 2016; Levi et al., 2019;
 88 Bao et al., 2019). However, for larger T , the $S(T)$ relation becomes very nonlinear so that S
 89 practically does not grow with T increase for $T > T_0$ (McQuillan, 1973; Ladeira & Price,
 90 1981; Sagy & Reches, 2006; Ji et al., 2021). This $S(T)$ relation was recently obtained in
 91 elastoplastic numerical models (Chemenda et al., 2021), where a progressive fracturing in the
 92 initially homogeneous models resulted from inelastic straining or damage of the material. At a
 93 certain stage, the damage localizes into narrow pure dilation deformation bands, leading to
 94 complete material failure that is fracture initiation. This process can involve the whole layer if
 95 T is sufficiently small, or only the parts near the interfaces with the adjacent layers if T is
 96 large. In the latter case, the fracture develops in two stages. The first one includes distributed
 97 layer damage in the vicinity of its horizontal boundaries, localization of this damage in bands,
 98 and fracture initiation. At the second stage, the initiated fracture propagates quasi-statically
 99 across the layer. These processes are the subject of a detailed study in this paper.



100 **Figure 2.** Setup of 3-layer models. (a) Series of alternating incompetent (pink) and competent
 101 (blue) layers. (b) An elementary (repeating) element of this series which corresponds to the

102 complete three-layer modeling setup. (c) A half-symmetry modeling setup, with thicknesses
103 of layers 1 and 2 being $T_1/2$ and $T/2$, respectively. V_x and V_z are the velocities applied in the
104 corresponding directions to layers 1 and 3. V_x causes deformation and fracturing of layer 2
105 and V_z is to maintain constant average vertical (lithostatic) stress at the horizontal model
106 boundaries. The y -normal model boundaries are fixed in the y -direction. The layers are
107 separated by cohesive-frictional interfaces. The models are pre-stressed in the y - and z -
108 directions as indicated below. Layers 1 and 3 are purely elastic and layer 2 is elastoplastic.
109 $T_1 = T_1 = 0.2$ m, $T = 1$ m, and $L = 0.6$ m.

110

111 Since fractures emanate from dilation localization bands, strain localization is a fundamental
112 element of fracture formation and should be accurately modeled. This process, resulting from
113 a constitutive instability and deformation bifurcation (Rice, 1976; Rudnicki & Rice, 1975), is
114 known to be strongly mesh-dependent in continuum numerical models (e.g., Needleman,
115 1988; Pijaudier-Cabot & Bažant, 1987), and therefore requires their regularization to reduce
116 the mesh dependence. In Chemenda et al. (2021), the reduction of mesh-dependence of the
117 modeling results was achieved by integrating the mesh size Δz into the constitutive
118 formulation so that the energy dissipation within the deformation/fracture bands is
119 independent on Δz . Since this procedure does not eliminate the ill-posedness of the initial
120 value problem during strain localization, the numerical scheme used might not be robust
121 enough to capture correctly the deformation banding that affects the following fracture
122 process. Different regularization techniques have been applied to deal with this issue,
123 including nonlocal/gradient (e.g., Chen & Schreyer, 1987; Needleman, 1988; Nguyen &
124 Korsunsky, 2008; Pijaudier-Cabot & Bažant, 1987; Poh & Swaddiwudhipong, 2009;
125 Vardoulakis, 1989) or viscous (Duvaut and Lions, 1972; Perzyna, 1996; Needleman, 1988;
126 Simo et al., 1988; Wang et al., 1997; Loret and Prevost, 1990) elastoplastic models. Viscous
127 regularization is the simplest, not expensive numerically, and widely used approach (e.g., Das
128 et al., 2013; Carosio et al., 2000; Heeres et al., 2002; Shahin, et al., 2019; Duretz et al., 2019),
129 which is also applied here.

130 Below we describe the constitutive model and the regularization aforisms used. We then
 131 present the mentioned above main three-layer (Fig. 2) and subsidiary, one-layer modeling
 132 setups. The latter is designed to investigate the details of dilation banding for different model
 133 parameters. We then present and discuss the modeling results obtained and give our
 134 conclusions.

135 2 Constitutive model

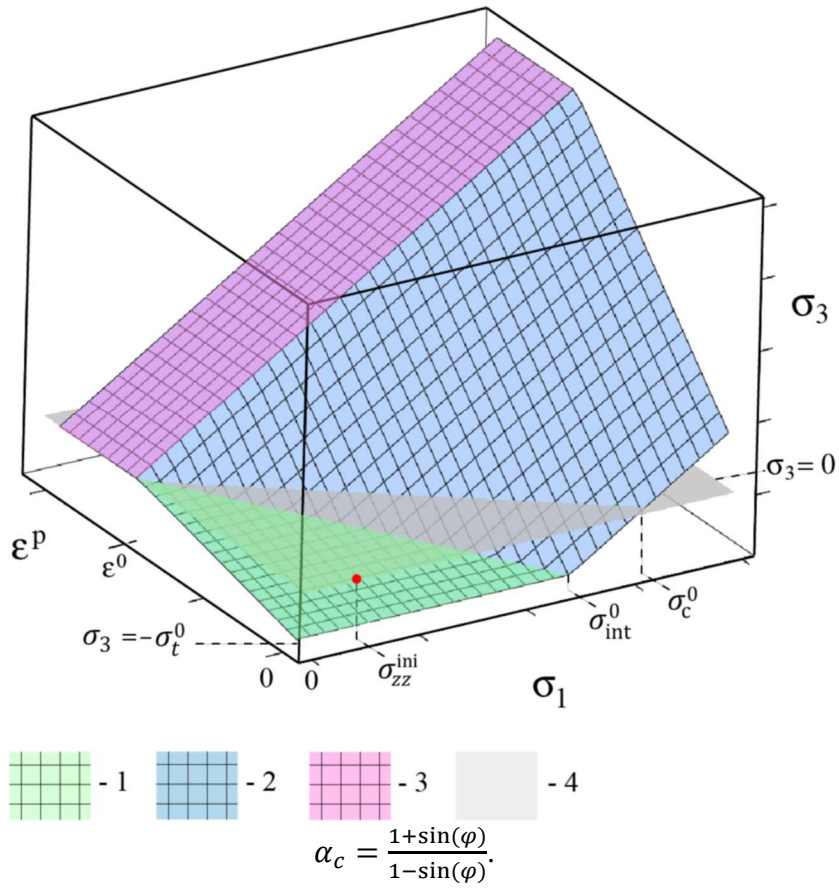
136 To model inelastic straining and fracture of layer 2 (Fig. 2), we use the constitutive model
 137 from Chemenda et al. (2021) summarized here. The model includes the following composite
 138 yield function

$$139 \quad F = \begin{cases} F_t = \sigma_t + \sigma_3 & \text{if } \sigma_1 \leq \sigma_{int} \\ F_s = \alpha_c \sigma_3 + \sigma_c - \sigma_1 & \text{if } \sigma_1 > \sigma_{int} \end{cases} \quad (1)$$

140 where F_t and F_s are the yield functions for the tensile and shear failure mechanisms,
 141 respectively; σ_t and σ_c are the tensile and unconfined compression strengths, respectively;
 142 σ_{int} is the abscise of the intersection point of the envelopes $F_t = 0$ and $F_s = 0$ in the
 143 $(\sigma_1, \sigma_3, \varepsilon^p)$ coordinates (Fig. 3), where ε^p is the accumulated inelastic volume strain tracking
 144 the history of inelastic strain. A rock mechanics convention is used for stresses: $\sigma_1 \geq \sigma_2 \geq \sigma_3$,
 145 where the compressive stress is positive, and tension is negative. All stresses are effective.
 146 The parameters σ_t , σ_c , and σ_{int} are functions of ε^p

$$147 \quad \sigma_t(\varepsilon^p) = \sigma_t^0 \kappa(\varepsilon^p), \quad \sigma_c(\varepsilon^p) = \sigma_c^0 \kappa(\varepsilon^p), \quad \sigma_{int}(\varepsilon^p) = \sigma_{int}^0 \kappa(\varepsilon^p) \quad (2)$$

148 where ε^0 is the ε^p value at which both tensile and compression strengths reach zero during
 149 failure; $\kappa(\varepsilon^p) = \max(0, (1 - \varepsilon^p/\varepsilon^0))$; σ_t^0 , σ_c^0 , and σ_{int}^0 are the initial (at $\varepsilon^p = 0$) values of
 150 σ_t , σ_c , and σ_{int} ; α_c is the dimensionless material (friction) parameter related to the Coulomb
 151 internal friction angle φ as



152

153

154 **Figure 3.** Composite yield surface $\sigma_3(\sigma_1, \varepsilon^p)$. (1) Tensile failure. (2) Shear failure. (3) Post
 155 failure (after complete failure). (4) Shows a zero-level of σ_3 . The red point (circle)
 156 corresponds to the initial stresses $\sigma_1 = \sigma_{xx}^{ini}$ and $\sigma_3 = 0$ applied to the models.

157

158 The tensile and shear failure mechanisms are thus coupled in this model by synchronous
 159 evolution of the strengths σ_t and σ_c during the inelastic straining; both reach zero at the same
 160 ε^p , $\varepsilon^p = \varepsilon^0$ (Fig. 3).

161 The plastic potential function Φ reads

$$\Phi = \begin{cases} \Phi_t = \sigma_3 & \text{if } \sigma_1 \leq \sigma_{int} \\ \Phi_s = \beta_c \sigma_3 - \sigma_1 & \text{if } \sigma_1 > \sigma_{int} \end{cases} \quad (4)$$

162

163 where Φ_t and Φ_s are the plastic potentials for the tensile and shear failure mechanisms,
 164 respectively; β_c is the material coefficient depending on ε^p and linearly decreasing from its
 165 initial value β_c^0 to 1 with ε^p

$$166 \quad \beta_c = \beta_c^0 + (1 - \beta_c^0)(1 - \kappa) \quad (5)$$

167 This coefficient defines the dilatancy factor $\beta = d\varepsilon^p / d\bar{\gamma}^p$, where $d\bar{\gamma}^p$ is the increment of
 168 inelastic equivalent or maximum shear strain. For the latter case

$$169 \quad \beta = \frac{\beta_c - 1}{\beta_c + 1}. \quad (6)$$

170 as can be obtained from (4, 5) and the flow rule

$$171 \quad d\varepsilon_i^p = d\lambda \frac{\partial \Phi_s}{\partial \sigma_i}, \quad (7)$$

172 where $d\lambda$ is the nonzero scalar function ($d\lambda$ is different for the different failure mechanisms
 173 introduced), $i = 1, 2, 3$. It follows from (6) that when $\beta_c = 1$, $\beta = 0$. We assume here that
 174 $\beta_c^0 = 1$, meaning no inelastic volume increase (change) during inelastic shear deformation.
 175 This increase can occur only when the tensile failure/damage mechanism is activated.

176 2.1 Integration of the mesh size into the constitutive formulation

177 To deal with the mesh-dependence of the results of fracture modeling, the mesh (numerical
 178 zone) size Δz is related to ε^0 as (Chemenda et al., 2021)

$$179 \quad \varepsilon^0 = \tilde{\varepsilon}^0 \left(\frac{C}{\Delta z} \right) \quad (8)$$

180 where C is a constant coefficient, and $\tilde{\varepsilon}^0$ is equal to ε^0 when $\Delta z = C$. This relation allows
 181 reducing the dependence on Δz of the rate of inelastic energy dissipation W within the
 182 deformation/fracture band during its extension. Indeed, as follows from (Eqs. 4 and 7), only
 183 the σ_3 -parallel component of inelastic strain is nonzero and is equal to ε^p during the tensile

184 failure. Assuming that inelastic straining within the band is uniform, that the band width d_0 is
 185 proportional to Δz ($d_0 \sim \Delta z$), and $\varepsilon^p = \Delta d/d_0 \sim \Delta d/\Delta z$, the energy dissipation rate W per unit
 186 height and thickness of the band can be written as

$$187 \quad W = \frac{d_0}{\Delta d} \int_0^{\varepsilon^p} \sigma_t(\varepsilon^p) d\varepsilon^p \sim \frac{\Delta z}{\Delta d} \int_0^{\Delta d} \sigma_t \left(\frac{\Delta d}{\Delta z} \right) \frac{d(\Delta d)}{\Delta z} = \sigma_t^0 \left[1 - \frac{\Delta d}{2\Delta z \varepsilon^0} \right] \quad (9)$$

188 W will be constant for a given Δd when $\Delta z \varepsilon^0$ is constant, which is equivalent to (8).

189 2.2 Viscous regularization

190 The procedure described above does not eliminate the loss of hyperbolicity or ellipticity of the
 191 field equations in dynamic or static regimes, respectively, which results in the ill-posedness of
 192 the initial value problem during instability leading to strain localization. To tackle this
 193 problem, we introduce viscosity into the constitutive formulation using Duvaut-Lions scheme
 194 (Duvaut and Lions, 1972) investigated notably by Loret and Prevost (1990). The resulting
 195 constitutive relations in small strain formalism read

$$196 \quad \dot{\sigma}_{ij} = 2G\dot{\varepsilon}_{ij} + \left(K - \frac{2}{3}G \right) \dot{\varepsilon}_{kk} \delta_{ij} - \frac{1}{\eta} (\sigma_{ij} - \bar{\sigma}_{ij}) H \left(F(\sigma_{ij}, \varepsilon^p) \right)$$

197 (10)

$$198 \quad \dot{\varepsilon}^p = -\frac{1}{\eta} (\varepsilon^p - \bar{\varepsilon}^p) H \left(F(\sigma_{ij}, \varepsilon^p) \right)$$

199 where σ_{ij} and ε_{ij} are the stress and strain tensors, respectively; $(\dot{\quad})$ and $(\bar{\quad})$ denote
 200 respectively the time derivative and the solutions of the inviscid problem; G and K are the
 201 shear and bulk elastic moduli, respectively; H is the Heaviside step function, and $\eta \geq 0$ is the
 202 nonnegative parameter with the dimension of time, called the relaxation time; $i, j, k = 1, 2, 3$.
 203 For $\eta = 0$, the rate-independent plasticity model is recovered $(\sigma_{ij}, \varepsilon^p) = (\bar{\sigma}_{ij}, \bar{\varepsilon}^p)$.

204 We have implemented the constitutive model (1, 2, 4, 5, 8, 10) into the finite-difference
 205 dynamic time-marching explicit code FLAC3D (Itasca, 2021), used in a quasi-static mode

206 (i.e., the steady-state solution of a fully dynamic problem is obtained by a dynamic relaxation
 207 method). In our implementation, we use the discrete approximation given by Simo et al.
 208 (1988), which can be summarized in the following steps. Assuming a constant strain
 209 increment $\Delta\varepsilon_{ij} = \varepsilon_{ij}\Delta t$ over the time interval $[t^n, t^n + \Delta t]$ between steps n and $n + 1$, we
 210 compute the elastic trial stress

$$211 \quad \sigma_{ij}^{tr} = \sigma_{ij}^n + 2G\Delta\varepsilon_{ij} + \left(K - \frac{2}{3}G\right)\Delta\varepsilon_{kk}\delta_{ij} \quad (11)$$

212 If $F(\sigma^{tr}, \varepsilon^{p^n}) < 0$, $(\sigma_{ij}^{n+1}, \varepsilon^{p^{n+1}}) = (\sigma_{ij}^{tr}, \varepsilon^{p^n})$, otherwise the inviscid back-bone solution
 213 $(\bar{\sigma}_{ij}^{n+1}, \bar{\varepsilon}^{p^{n+1}})$ is first computed by projecting the stress state onto the current yield surface.
 214 Then (10) is integrated using the Euler backward scheme to obtain the visco-elastoplastic
 215 solution (update/correction of σ_{ij} and ε^p).

$$216 \quad \sigma_{ij}^{n+1} = \frac{1}{1+\gamma}(\sigma_{ij}^{tr} + \gamma\bar{\sigma}_{ij}^{n+1}), \quad \varepsilon^{p^{n+1}} = \frac{1}{1+\gamma}(\varepsilon^{p^n} + \gamma\bar{\varepsilon}^{p^{n+1}}) \quad (12)$$

217 where the only new parameter is $\gamma = \Delta t/\eta$. This dimensionless nonnegative parameter
 218 influences the inelastic deformation in an opposite way to the classical viscosity coefficient.
 219 The viscosity effect is maximum when $\gamma \rightarrow 0$, and $\gamma = 0$ corresponds to purely elastic
 220 behavior. The viscosity effect is inexistent when $\gamma = \infty$, which corresponds to a purely
 221 elastoplastic or inviscid model.

222 **2 Modeling setup**

223 **2.1 Three-layer models**

224 As in the previous studies cited in the Introduction, we investigate a three-layer model shown
 225 in Fig. 2b. Layers 1 and 3 are subjected to the horizontal extension, generating shear stresses
 226 at the layer interfaces driving the extension and fracturing of the central layer 2. This layer has
 227 free vertical boundaries that can be considered preexisting, previously formed fractures. The

228 whole model is pre-stressed to the initial stresses σ_{zz}^{ini} , σ_{yy}^{ini} , and σ_{xx}^{ini} . The horizontal
 229 extension applied to the model causes its vertical shortening. To maintain the average vertical
 230 stress constant and equal to σ_{zz}^{ini} , we apply servo-controlled vertical velocities V_z to the
 231 horizontal boundaries of the models (Fig. 2b).

232 The layers are connected by frictional and cohesive interfaces whose shear strength τ_0^{int} is
 233 defined by the interface friction coefficient μ^{int} and cohesion c^{int}

$$234 \quad \tau_0^{int} = \mu^{int} \sigma_n + c^{int} \quad (13)$$

235 where σ_n is the effective normal to interface stress which is equal to the normal vertical stress
 236 σ_{zz} . The normal (k_n) and shear (k_s) stiffnesses of the interfaces are set to (Itasca, 2021)

$$237 \quad k_n = k_s = 10 \max \left[\frac{4G+3K}{3\Delta z} \right] \quad (14)$$

238 where "max" means that the maximum value over all zones adjacent to the interface is to be
 239 used.

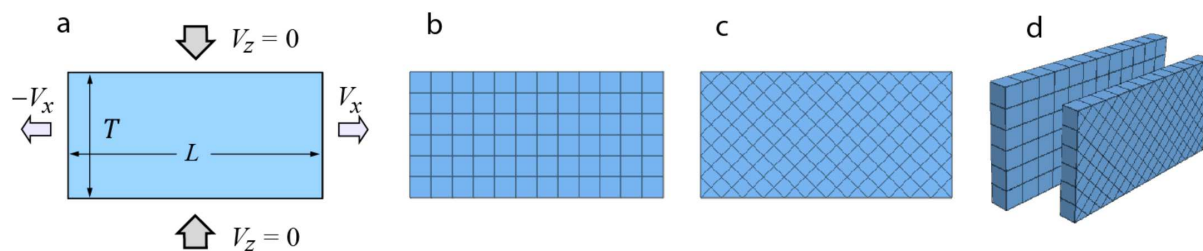
240 Fig. 2b shows the complete modeled structure, but to reduce the calculation time, the
 241 simulations have been carried out with the half-symmetry setup in Fig. 2c.

242 2.2 One-layer models

243 Before three-layer modeling, we investigate the setup in Fig. 4a with one elastoplastic layer
 244 subjected to the uniaxial extension. These models with simple geometry and uniform loading
 245 and straining conditions correspond to the theoretical framework of the analysis of
 246 deformation localization (bifurcation) that results from a constitutive (or material) instability
 247 (Rice, 1976). They are designed to investigate this phenomenon in a specific regime
 248 corresponding to pure dilation banding and to compare the results against the relevant
 249 theoretical predictions (Ottosen & Runesson, 1991). Particular attention is given to

250 understanding the impact of the regularization algorithms presented on strain localization and
 251 studying the influence of the numerical grid geometry and structure shown in Figs. 4b–4d on
 252 the localization. The double sheet brick-wedge grid in Fig. 4d consists of the attached brick-
 253 and wedge-shaped grids shown in Figs. 4b and 4c. The attachment procedure consists of a
 254 rigid attachment (or slaving) of the gridpoints of one zone to the opposite, master gridpoints,
 255 faces, or edges by imposing to the slave gridpoints of velocities/displacements obtained from
 256 those in the three or four grid points that make up the master face. Forces are distributed from
 257 the slave to the master gridpoints. The velocities obtained from the equations of motion at
 258 each step are transferred from the master to the slave gridpoints using weighting values
 259 (Itasca, 2021).

260 When the layer model has a strictly rectangular (parallelepipedal) shape and uniform
 261 properties, its extension leads to the formation of pure dilation deformation bands along one
 262 or both vertical borders. A small zone of a very small weakness is usually imposed at the
 263 model center to avoid these boundary effects. Another way, which we preferred in this study,
 264 is a very small progressive (sinusoidal) thinning of the model (plate) with the maximum
 265 amplitude of $1\ \mu\text{m}$ in its central part.



266 **Figure 4.** Setup of one-layer models (a) and grid geometries used (b to d). (b and c) Brick-
 267 and wedge-shaped grids, respectively. (d) Double-layer sheet grid, with the attached brick and
 268 wedge-shaped grids. $T = 0.1\ \text{m}$, and $L = 0.2\ \text{m}$.

269

270 3 Modeling results

271 The results are organized below into five groups addressing different aspects of strain
 272 localization and fracture. The first four groups include one-layer models (setup in Fig. 4a),
 273 and the two next ones present three-layer models (Fig. 2b) run using a half-symmetry setup in
 274 Fig. 2c.

275 The deformation localization and fracture patterns are shown in terms of the tensile strength
 276 σ_t . When σ_t is equal to its initial value $\sigma_t^0 = 7$ MPa, there is no material damage, and when
 277 $\sigma_t = 0$, the material is wholly fractured/failed. The case $0 < \sigma_t < \sigma_t^0$ corresponds to the
 278 dilatant damage of the material. Localization of such damage within a narrow band
 279 corresponds to pure dilation banding, which can evolve to fracture with the following damage
 280 accumulation. Since the only elastoplastic layer (layer 2 in Fig. 2) can fracture, only this layer
 281 is shown in the figures presenting the results from 3-layer models.

282 The deformation stages are characterized by the nominal normal horizontal extension strain
 283 $\varepsilon_{xx} = -\Delta L/L$, where L is the model length, and ΔL is its horizontal lengthening. In 1-layer
 284 models, ε_{xx} (or more precisely, V_x) is applied to the vertical borders of the layer (Fig. 4a), and
 285 in 3-layer models, only to layers 1 and 3 (Fig. 2b). The nominal horizontal stress σ_{xx} in the
 286 stress-strain curves presented below for 1-layer models is the average over the layer thickness
 287 normal stress in the x -direction.

288 We use here the model parameter values assumed and justified in Chemenda (2019) and
 289 Chemenda et al. (2021). The parameter values common for all models are $E = 20$ GPa; $\nu =$
 290 0.25 ; $\sigma_c^0 = 60$ MPa, $\sigma_t^0 = 7$ MPa, $\alpha_c = 3$, $\beta_c^0 = 1$, $C = 0.1$ m, $\rho = 2600$ kg/m³, $\sigma_{zz}^{ini} =$
 291 10 MPa, $\sigma_{yy}^{ini} = \sigma_{zz}^{ini}/2$. In 1-layer models: $L = 0.2$ m, $T = 0.1$ m, $V_x = 1 \times 10^{-10}$ m/s, and
 292 $\sigma_{xx}^{ini} = -6.97$ MPa, which is set close to $-\sigma_t^0$ to approach the failure point and reduce the
 293 time for the purely elastic loading. For 3-layer models: $T_1 = T_3 = 0.2$ m, $T = 1$ m, $L = 0.6$ m
 294 (see Fig. 2a for definitions), $c^{int} = \tau_0^{int} = 4$ MPa, $k_n = k_s = 9.6 \times 10^{12}$ Pa/m (calculated

295 from (14)), $\sigma_{xx}^{ini} = 0$, $V_x = 5 \times 10^{-9}$ m/s. Other parameters: Δz , ε^0 , and γ , are varied in the
 296 models of different groups and are given in the captions of corresponding figures. For the
 297 chosen $\sigma_{zz}^{ini} = \sigma_1$ value, inelastic straining starts in the tensile failure domain, as can be seen
 298 in Fig. 3 (red circle). Therefore, the localization of strain (damage) should occur at negative
 299 hardening modulus (which is the case in our models) in the form of pure dilation bands
 300 oriented normal to σ_3 (Ottosen & Runesson, 1991; Chemenda, 2019).

301 Given that stresses are effective and assuming that the pore pressure is equal to the hydrostatic
 302 pressure, the lithostatic stress σ_{zz}^{ini} is related to the depth z as

$$303 \quad \sigma_{zz}^{ini} = (\rho - \rho_w)gz = 640 \text{ m} \quad (15)$$

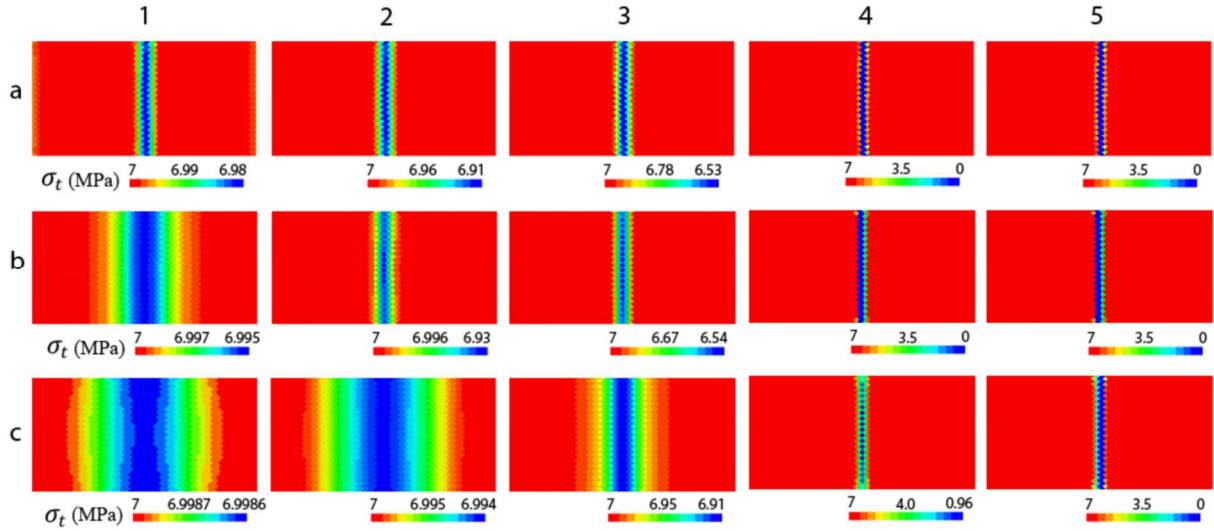
304 where $\sigma_{zz}^{ini} = 10$ MPa, $\rho_w = 10^3$ kg/m³ is the water density, and g is the acceleration of
 305 gravity.

306

307 3.1 Pure dilation banding in a layer under uniaxial horizontal extension

308 *Group 1: Impact of the viscosity parameter γ on the initiation and evolution of strain*
 309 *localization.*

310 Fig. 5 shows five deformation stages (columns 1 to 5) in three models (lines a to c) for
 311 different γ , decreasing from a to c. One can see that the higher the viscosity (the lower the γ
 312 value), the slower the strain localization and the wider the dilation bands at the initial stages
 313 of their evolution. There is, however, no fundamental difference between the models and the
 314 width d_0 of final band/fracture zones (column 5): it is practically the same and equal to $\sim \Delta z$.
 315 As expected, the deformation bands are normal σ_3 (horizontal in Fig. 5) and hence parallel to
 316 σ_1 , which is vertical in the figure. Therefore, the obtained deformation bands are pure dilation
 317 bands, which is also confirmed by the orientation of the velocity field within them.



318

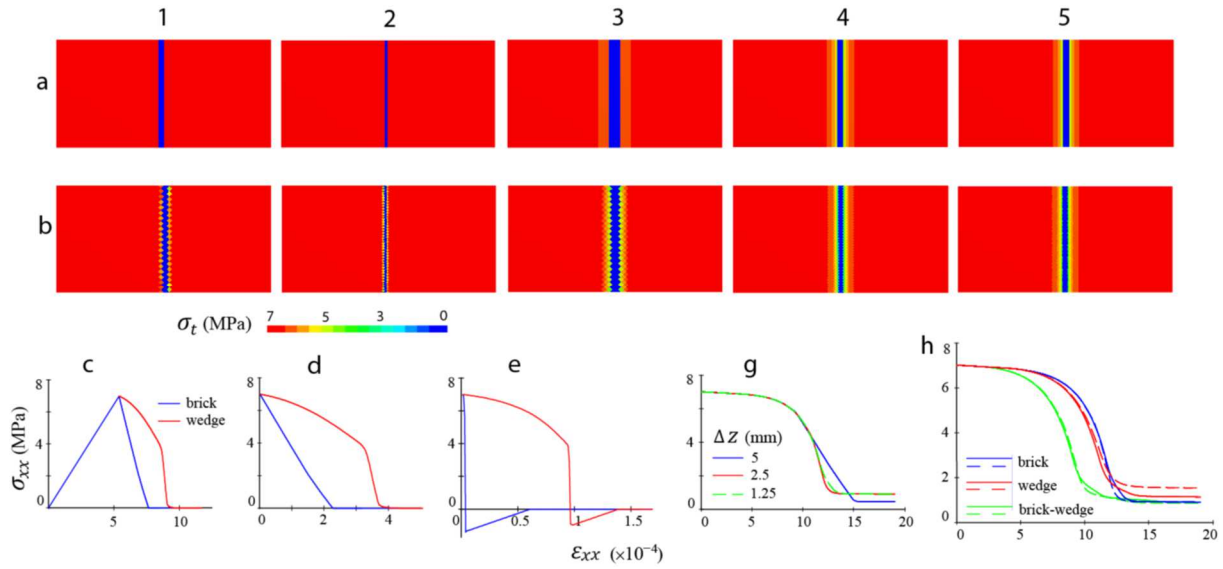
319 **Figure 5.** Group 1. Evolution of strain localization and fracture (stages/columns 1 to 5) in
 320 three models (a to c) differing only by the γ value: in (a), $\gamma = \infty$; in (b), $\gamma = 0.1$, and in (c),
 321 $\gamma = 0.01$. Deformation stages 1 to 5 correspond to ϵ_{xx} equal to -5×10^{-6} , -1.5×10^{-5} ,
 322 -6×10^{-5} , -4.5×10^{-4} , and -7.8×10^{-4} , respectively. $\Delta z = 5$ mm and $\epsilon^0 = 0.02$. All the
 323 models have wedge-shaped grids shown in Fig. 4c.

324

325 *Group 2:* Dependence of the dilation banding and fracture on the grid geometry and resolution
 326 in the inviscid and viscous models

327 Fig. 6 shows the final stages of strain localization corresponding to the complete failure of the
 328 material in ten models with brick- (Figs. 6a) and wedge- (Figs. 6b) shaped meshes with
 329 different resolutions specified in the figure caption. The models in columns 1 and 2 are
 330 inviscid ($\gamma = \infty$), and in the models in columns 3 to 5, $\gamma = 1 \times 10^{-3}$. In the inviscid models,
 331 the deformation/fracture band width d_0 is equal to $\sim \Delta z$. In the viscous models (columns 3–5),
 332 d_0 includes several grid elements. Their number increases with the Δz reduction so that d_0
 333 remains constant (Δz –independent) for sufficiently small Δz , $\Delta z < \sim 4$ mm. Therefore, the
 334 introduction of sufficiently small γ (large viscosity) regularizes the problem in the sense that
 335 d_0 becomes independent of both the grid resolution and geometry. This is true not only for the
 336 brick- and wedge- (compare images in columns 4 and 5), but also for double brick-wedge
 337 grids shown in Fig. 4d. The structural stress-strain responses also converge with Δz reduction

338 (Fig. 6g), although they are different for different grids (Figs. 6h). The $\sigma_{xx}(\varepsilon_{xx})$ curves for the
 339 inviscid models are different (Figs. 6c to 6e) and attest to more brittle behavior, with the
 340 brittleness increasing as Δz decreases (compare Figs. 6d and 6e).



341

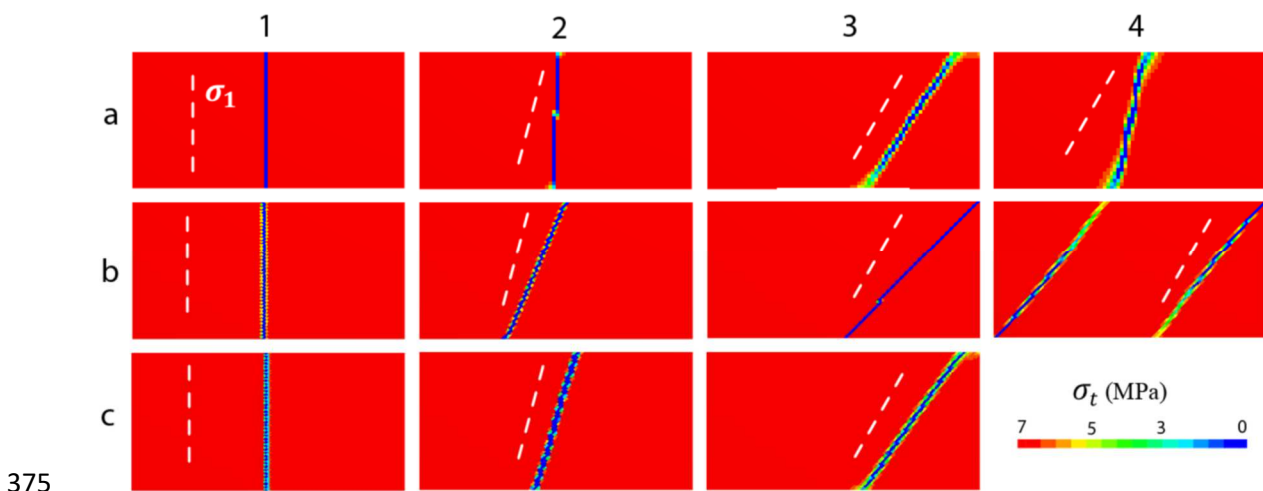
342 **Figure 6.** Group 2. Impact of the grid geometry, resolution, and the regularization parameter
 343 γ on the dilation banding and structural stress-strain response. Final stages of strain
 344 localization and fracture are shown for five models with brick- (a) and wedge-shaped (b)
 345 meshes, respectively. The resolution of the models in columns 1 and 3 is $\Delta z = 5$ mm, in
 346 columns 2 and 4, 2.5 mm, and in column 5, 1.25 mm. In columns 1 and 2, $\gamma = \infty$, and in
 347 columns 3 to 5, $\gamma = 1 \times 10^{-3}$. (c to h) Nominal stress-strain curves $\sigma_{xx}(\varepsilon_{xx})$ in the presented
 348 models. Since the models are prestressed to σ_{xx} close to $-\sigma_t^0$, the curves start near the initial
 349 failure (yield) point except in (c), where the elastic loading stage (segment) is added to the
 350 curves in (d). The curves in (d and e) are respectively for the models in columns 1 and 2
 351 (curve (c) is for column 1 as well). Curves in (g), are for the regularized brick-shaped models
 352 in (a3 to a5) with different resolutions indicated on the plot. (h) Curves for the regularized
 353 models with the brick, wedge, and double brick-wedge grids corresponding to the curves of
 354 different colors as indicated in (h). Solid curves are for $\Delta z = 1.25$ mm, and the dashed ones,
 355 for $\Delta z = 2.5$ mm.

356

357 *Group 3:* Impact of the grid geometry on the orientation of deformation bands and the
 358 resulting fractures.

359 The pure dilation bands in our models (given the constitutive framework used and the stress
 360 values applied) should form normal to σ_3 and parallel to σ_1 and σ_2 . However, the grid

361 geometry can also affect the band orientation (as well as its width) in the numerical models.
 362 When σ_1 is parallel to a grid line, the band is parallel to this line as can be seen in Fig. 7a1 (all
 363 models in Fig. 7a have brick-shaped meshes shown in Fig. 4b). The dilation bands and
 364 resulting fracture bands remain parallel to the grid line (vertical in Fig. 7), even when the σ_1
 365 orientation deviates from this line provided that the deviation angle ψ does not exceed a
 366 certain value. In Fig. 7a2, $\psi = 15^\circ$, but the final deformation/fracture band is still vertical. In
 367 Fig. 7a3, $\psi = 30^\circ$ and the band is inclined (but not parallel to σ_1). In this case d_0 is $\sim 1.5\Delta z$,
 368 whereas in Figs 7a1 and Figs 7a2 where the bands are parallel to the grid lines, $d_0 = \Delta z$. It
 369 was expected that in the regularized models, the orientation of the fracture bands would be
 370 closer to σ_1 ; however, this is not the case (Fig. 7a4). Similar conclusions can be drawn from
 371 the models in Figs. 7b with wedge-shaped grids. On the contrary, the models with the double-
 372 layer grids provide more satisfactory results (Fig. 7c) both in terms of the band thickness
 373 (which is practically the same, $d_0 \approx 1.5\Delta z$, for different ψ) and orientation. This orientation
 374 further approaches that of σ_1 with the mesh refinement.

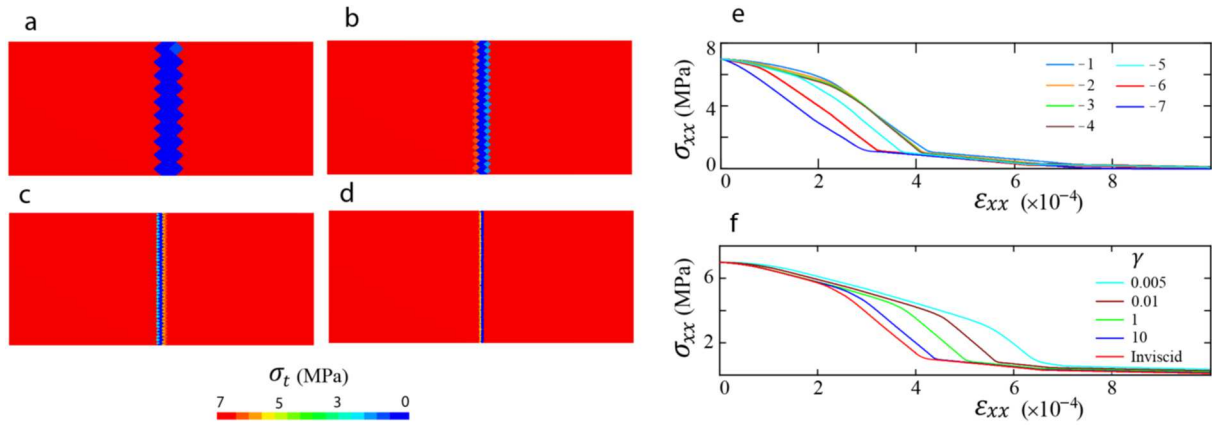


376 **Figure 7.** Group 3. Final stages of strain localization and fracture in the models with brick (a),
 377 wedge (b), and double brick-wedge (c) grids. The columns 1 to 3 correspond to different
 378 orientations of the initial stress axes defined by angle ψ between σ_1 (shown by the white
 379 dashed lines) and the vertical; ψ is 0° , 15° , and 30° in columns 1, 2, and 3, correspondingly.
 380 In column 4, $\psi = 30^\circ$. The rotation of the initial stress axes is achieved by imposing the

381 corresponding normal and shear initial and boundary stresses. Models in columns 1 to 3 are
 382 inviscid ($\gamma = \infty$), and in column 4, $\gamma = 1 \times 10^{-3}$. In all models $\Delta z = 2.5$ mm and $\varepsilon^0 = 0.02$.
 383

384 The presented results show that although the viscous models exhibit clear regularization
 385 effects on the strain localization and band formation, they do not provide satisfactory results
 386 on the geometry and orientation of the fracture bands (Fig. 7a4 and 7b4) or the stress-state
 387 during and after the fracture formation. Indeed, the residual viscous horizontal tensile stress
 388 after the complete fracture (complete material failure) is $\sigma_{xx} \approx -1.2$ MPa on average in Fig.
 389 6h, whereas it should be zero in reality. The magnitude of this stress can be reduced by
 390 decreasing the viscous effect, i.e., by increasing γ . However, the increase of γ requires a rapid
 391 growth of the model resolution (reduction of Δz) to achieve a stabilization of both d_0 and the
 392 stress-strain response. For example, for $\gamma = 1 \times 10^{-3}$ applied in the models in Figs. 6a3–6a5
 393 and b3–b5, the stabilization starts at $\Delta z \approx 4$ mm, whereas for $\gamma = 1 \times 10^{-2}$ (still
 394 corresponding to high viscosity) it occurs at $\Delta z \approx 0.8$ mm. Such resolution is too high for
 395 most real-life applications. The viscous effects become negligible at much larger γ , $\gamma \approx 10$ as
 396 seen hereafter (Fig. 8f). This increases the attractiveness of using the double-layer grid in Fig. 4d
 397 with sufficiently large γ (low viscosity) needed only to ensure the well-posedness of the
 398 initial value problem. In this case, one has to give up the convergence of d_0 to a certain value
 399 that in any case cannot be realistic (very small), as will be discussed below. To ensure the
 400 independence of the energy dissipation on Δz within deformation bands during fracture, ε^0
 401 should be related to Δz by Eq. (8). This has been done in the models of the next group.

402 *Group 4:* Dilation banding and fracture in a layer in the models with different ε^0 (or
 403 hardening modulus) and Δz .



404

405 **Figure 8.** Group 4. (a to d) Final stages of strain localization and fracture in the inviscid
 406 models with double brick-wedge grids and different ϵ^0 and Δz related by Eq. (8): (a) $\epsilon^0 =$
 407 0.01 and $\Delta z = 10$ mm; (b) $\epsilon^0 = 0.02$ and $\Delta z = 5$ mm; (c) $\epsilon^0 = 0.04$ and $\Delta z = 2.5$ mm; (d)
 408 $\epsilon^0 = 0.08$ and $\Delta z = 1.25$ mm. (e) Nominal stress-strain curves from the models presented
 409 and other similar ones with different Δz (and hence ϵ^0): for (1) $\Delta z = 0.625$ mm; (2) $\Delta z =$
 410 1.25 mm; (3) $\Delta z = 2$ mm; (4) $\Delta z = 2.5$ mm; (5) $\Delta z = 2.7$ mm; (6) $\Delta z = 5$ mm; (7) $\Delta z = 10$
 411 mm. (f) Nominal stress-strain curves obtained from other models with $\Delta z = 1.25$ mm, $\epsilon^0 =$
 412 0.08 , and different γ indicated on this figure.

413

414 Figs. 8a–d show the fracture bands resulting from strain localization and evolution of pure
 415 dilation deformation bands in the double brick-wedge-grid models with different Δz and ϵ^0
 416 related by Eq. (8). As expected, the final band thickness d_0 decreases linearly with the Δz
 417 decrease. On the contrary, the stress-strain curves in Fig. 8e become very close for $\Delta z < 2.5$
 418 mm. These models are inviscid, i.e., $\gamma = \infty$. Reduction of γ , leads to the increase in the
 419 viscous stresses, reduction of the average viscoplastic hardening modulus (Fig. 8f), and
 420 increase in the dissipation energy. All these effects become negligible when γ is sufficiently
 421 large, larger than ~ 10 (Fig. 8f). For such γ values, the evolution of strain localization and
 422 fracture is practically the same as in the inviscid models. For smaller γ , the localization of
 423 deformation is more progressive, as can be seen in Fig. 5, and will be demonstrated below in
 424 the models of group 6. The models of this group and those of group 5 were conducted using
 425 the setup in Fig. 2c corresponding to the fracturing within layered rocks in the heterogeneous
 426 stress and strain fields and jointing in sedimentary basins as described in the Introduction.

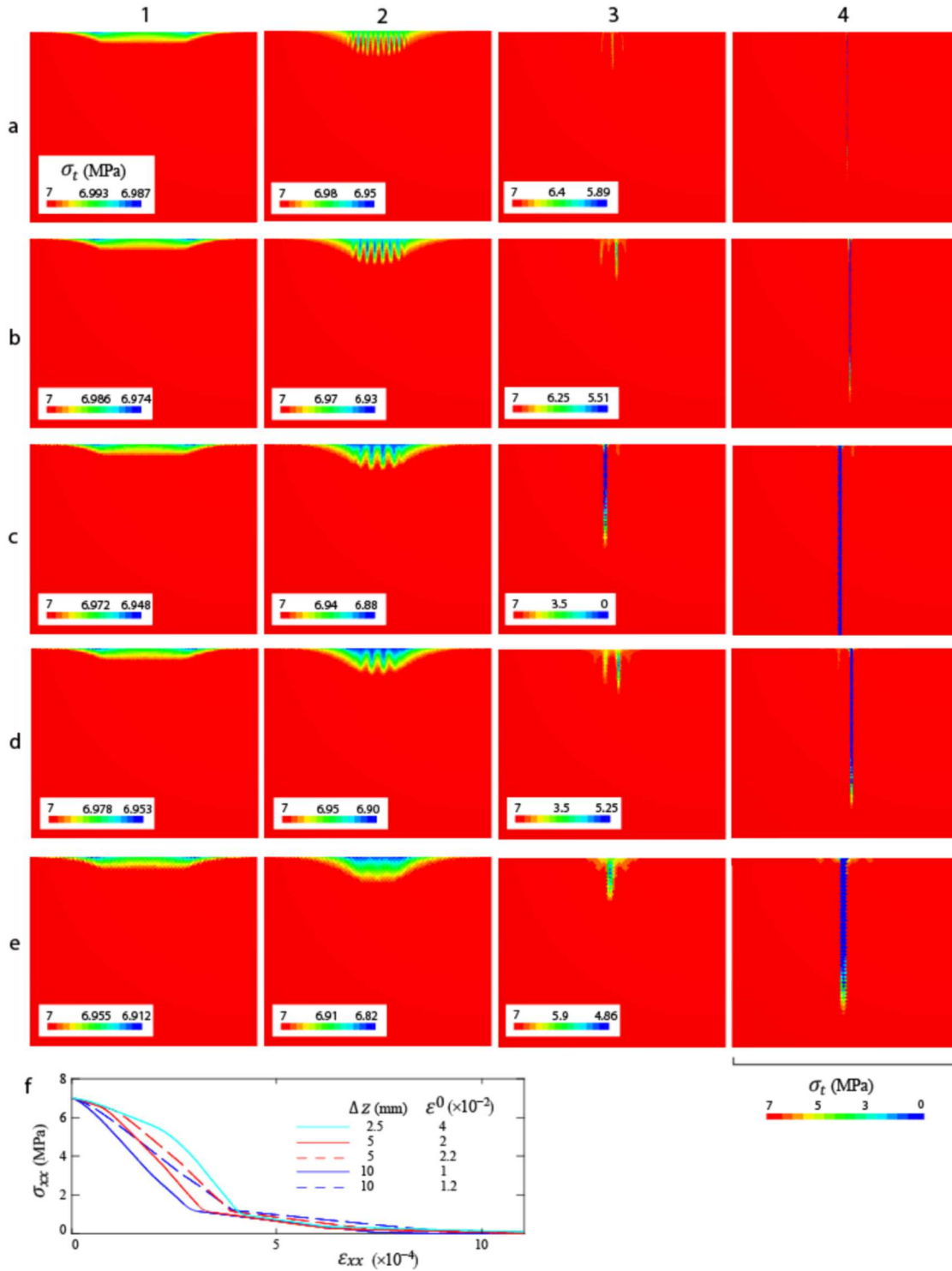
427 *Group 5: Fracturing of a thick inviscid elastoplastic layer embedded between the stretching*
 428 *elastic layers.*

429 Figs. 9a–e show four stages (columns 1 to 4) of the evolution of strain localization and
 430 fracture within the elastoplastic layer (the elastic layer is not shown) in five models with
 431 different Δz and ε^0 given in the figure caption. In the models in Figs. 9a–c, Δz and ε^0 are
 432 related by Eq. (8). The results are therefore supposed to be the same or close. This is indeed
 433 the case for the models with higher resolution $\Delta z = 1.25$ mm and $\Delta z = 2.5$ mm respectively
 434 in Figs. 9a and 9b, but the model in Fig. 9c with $\Delta z = 5$ mm shows more brittle behavior,
 435 with the fracture cutting through the entire layer at deformation stage 4 characterized by the
 436 same for all the models ε_{xx} value. This is not surprising as the response of the models
 437 becomes Δz -independent for Δz lower than a certain value. For the one-layer models, this
 438 value is around 2.5 mm (Fig. 8e), which is close to that following from Figs. 9a–c for the
 439 three-layer models that are characterized by different sizes and loading conditions (compared
 440 to one-layer models). For $\Delta z > 2.5$ mm, the stress reduction with the ε_{xx} increase is more
 441 rapid than for the models with smaller Δz as is seen in Fig. 8e. Therefore, the hardening
 442 modulus is more negative, and the fracture energy is smaller. To approach these parameters to
 443 the models with higher resolution, we increase ε^0 from 0.02 in Fig. 9c to 0.022 in Fig. 9d. The
 444 stress-strain curve for this ε^0 in one-layer models is closer to the curves for higher model
 445 resolution (Fig. 9f), and the strain localization and fracture processes in the three-layer model
 446 (Fig. 9d) approach those in Figs. 9a, b with higher resolution. In the lowest resolution model
 447 in Fig. 9e ($\Delta z = 10$ mm), $\varepsilon^0 = 0.012$ instead of 0.01 following from (8), for which the
 448 hardening modulus in the one-layer model is too negative (Fig. 9f). For $\varepsilon^0 = 0.012$, the
 449 $\sigma_{xx}(\varepsilon_{xx})$ curve is closer to those for smaller Δz (Fig. 9f). The result of strain localization and
 450 fracture in Fig. 9e4 is closer to that in higher resolution models in Figs. 9a4, b4, and d4 as

451 well. The difference between all these models is obviously in the d_0 values, but also in the
452 onset of strain localization near the layer interfaces. In Fig. 9a2, one can see many (14)
453 deformation bands, and in Fig. 9e2, none, but this has very little effect on the final result.
454 Note that the material damage at stage 2 is very small; the σ_t reduction is only $\sim 1\%$ of its
455 initial value σ_t^0 .

456 *Group 6:* Influence of the viscosity (regularization) on the evolution of strain localization and
457 fracture in the layered models.

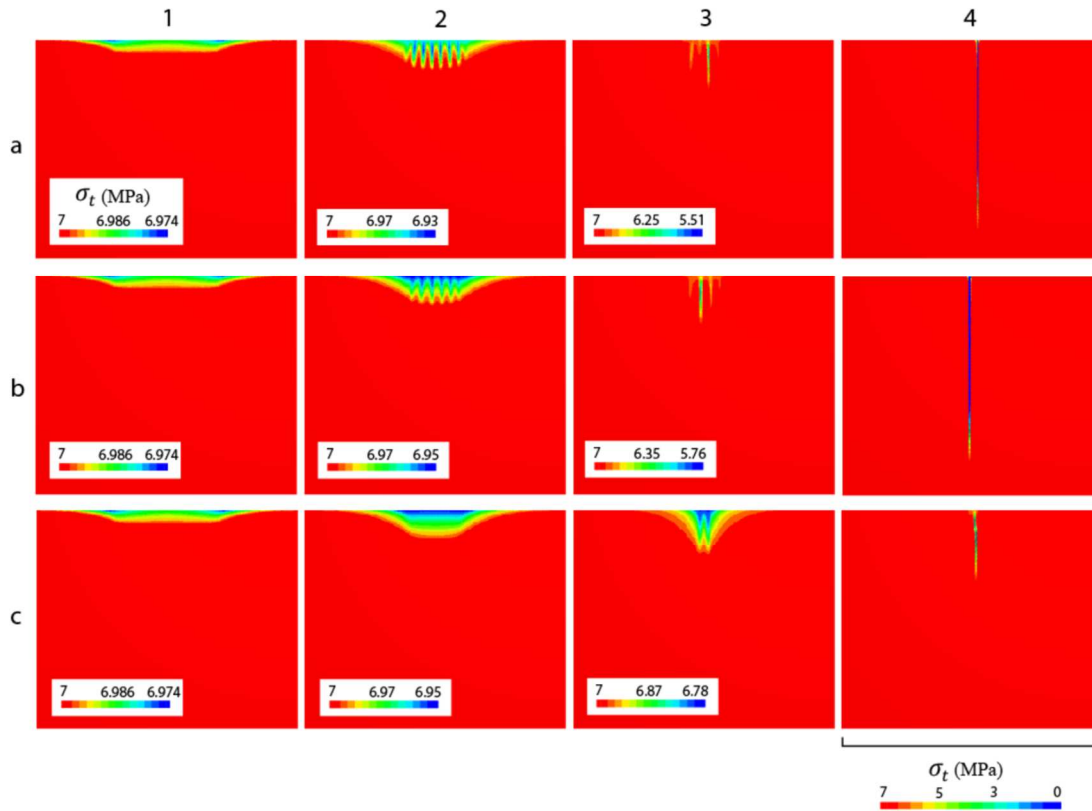
458 The setup and presentation of the results in Fig 10 are the same as for the models of the
459 previous group. All models have the same $\Delta z = 2.5$ mm and $\varepsilon^0 = 0.04$. They differ only in
460 the γ value: in Fig. 10a, which is the same as Fig. 9b, $\gamma = \infty$ and in Figs. 10b and 10c, γ is
461 0.15 and 0.01, respectively. One can see that in Fig. 10b2, the inelastic deformation is more
462 diffuse, and there are fewer deformation bands than in Fig. 10a2, although the fracture
463 evolution/propagation is practically the same at all stages. In the model in Fig. 10c, the



464

465 **Figure 9.** Group 5. Four evolutionary stages (columns 1 to 4) of strain localization and
 466 fracture in five 3-layer inviscid models (lines a to e) with double brick-wedge grids for layer
 467 2; only this layer (its half, Fig. 2c) is shown. The models differ only by Δz and ϵ^0 ; in (a to c),
 468 they are related by Eq. (8): (a) $\Delta z = 1.25$ mm, $\epsilon^0 = 0.08$; (b) $\Delta z = 2.5$ mm, $\epsilon^0 = 0.04$; (c)
 469 $\Delta z = 5$ mm, $\epsilon^0 = 0.02$. In (d), $\Delta z = 5$ mm, $\epsilon^0 = 0.022$, and in (e), $\Delta z = 10$ mm, $\epsilon^0 =$
 470 0.012 . The deformation stages shown (columns 1 to 4) correspond respectively to ϵ_{xx} of
 471 -6×10^{-4} , -9×10^{-4} , -2.1×10^{-3} , and -6×10^{-3} . (f) The stress-strain curves obtained
 472 from one-layer models for the same Δz and ϵ^0 as in the models a to e in this figure (the solid-
 473 line curves are the same as the corresponding curves in Fig. 8e).

474 viscous effect is the highest, and therefore there is no band initiation at stage 2 at all. It occurs
 475 only at stage 3, and so, the resulting fracture propagates over a much shorter distance. This
 476 fracture propagates over the same distance as in other models at larger ϵ_{xx} .



477

478 **Figure 10.** Group 6. Four evolutionary stages (columns 1 to 4) of strain localization and
 479 fracture in three 3-layer models (lines a to c) with double brick-wedge grids for the shown
 480 layer 2. The models differ only in the γ value: it is ∞ , 0.15, and 0.01 in (a, b, and c),
 481 respectively. In all models $\Delta z = 2.5$ mm, $\epsilon^0 = 0.04$; the deformation stages (1 to 4)
 482 correspond to the same ϵ_{xx} values as in the previous figure (see caption of Fig. 9).

483

484 6 Discussion

485 The width d_R of deformation localization bands in rocks at the origin of the faults and
 486 fractures is typically less than a fraction of a millimeter (subscript R stands for real/natural).

487 Numerical models of deformation banding with the numerical size of $N = 10^7$ can be

488 qualified as large or even very large. If size l of the modeled object (rock mass or geological

489 structure) is 10 m, then the numerical element (zone) size is $\Delta z = l/\sqrt[3]{N} = 4.6$ cm for the
 490 indicated N value. The width of deformation bands d_M in the numerical models is typically
 491 larger than Δz and hence much larger than d_R , $d_M \gg d_R$ (subscript M is for model). Since l
 492 can be hundreds of meters and kilometers, it is impossible to obtain deformation bands with
 493 realistic widths in most cases. Therefore, the convergence of the band thickness in numerical
 494 models like those in this study to a certain value using regularization procedures has a limited
 495 sense since this value will be very far from a realistic one anyway. On the other hand, such a
 496 convergence requires further model resolution refinement, as shown here. Therefore, one
 497 must accept that d_M is larger (much larger) than d_R and renounce the convergence of the band
 498 thickness with the model refinement. When using a viscous regularization like that in this
 499 paper, the introduction of a small viscosity (large γ) suffices to avoid the ill-posedness of the
 500 initial boundary value problem, although even this was not necessary for the models presented
 501 (compare, for instance, models in Figs. 10a and 10b). The effect of regularization should
 502 depend on the numerical code used and the details of numerical implementation. The dynamic
 503 relaxation procedure in FLAC3D, for example, provides a very diffusive integration scheme
 504 allowing to avoid the elastic structural snap backs during localization for any model
 505 refinement.

506 Since $d_M \neq d_R$, the constitutive model used in the numerical simulations cannot be exactly
 507 the same as that corresponding to natural material and defined from experimental data. It
 508 should be calibrated so that the energy dissipation during deformation localization and
 509 fracturing in the model is the same as in nature/experiment. Following Eq. (8), this means that
 510 ε^0 in the model (ε_M^0) should be related to the corresponding value ε_R^0 for nature as $\varepsilon_R^0/\varepsilon_M^0 \sim d_M/d_R$.
 511

512 The models in Figs. 9 and 10 correspond to a step in the sequential fracture infill in a
513 competent layer sandwiched between incompetent layers when a new joint forms between
514 two previously formed ones. The fracture initiation is preceded by the defused (stage 1 in
515 Figs. 9 and 10) and then localized inelastic straining or damage within several initial pure
516 dilation bands (stages 2 to 3), whose number depends on the model resolution (Fig. 9) and
517 viscosity (Fig. 10). It remains unclear if these bands do form in reality and, if yes, how many
518 they are. They can hardly be detected experimentally given a very low degree of material
519 damage within these bands (the strength reduction there does not exceed ~1%). The number
520 of the bands in the numerical models does not impact the following fracture initiation and
521 propagation processes. Therefore, the inelastic strain in the central oval zones near the layer
522 interfaces (stage 2 in Figs. 9 and 10) can be considered diffusive until its definitive
523 localization within a propagating band (stage 3) evolving to fracture initiation and
524 propagation from the layer interface to the layer center (stage 4). Note that both geological
525 observations ((Helgeson and Aydin, 1991; Savalli and Engelder, 2005; de Jussineau et al.,
526 2005)) and experimental studies (Jorand et al., 2012; Chemenda, 2019) confirm that the
527 fractures typically initiate from the interfaces of the fractured layer.

528 The models in Figs. 9 and 10 allow us to appreciate the limits of the most common tool used
529 to analyze and predict the jointing in the rocks, Linear Elastic Fracture Mechanics. This
530 theory implicitly assumes inelastic straining only in a very small zone at the tip of the
531 imposed initial crack or seed oriented in a "right" (vertical in the context of Figs. 9 and 10)
532 direction. In the modeling approach proposed here, the initial defect or weak zone is not
533 imposed but formed with the orientation defined by the local stress field.

534 **7 Conclusions**

535 The fracturing of layered rocks with contrasting mechanical properties typical for sedimentary
536 piles (basins) occurs in the brittle (competent) layers due to the tangential tractions generated
537 at the frictional-cohesive interfaces between the adjacent layers. The fracturing process starts
538 from inelastic straining or damage that should localize at a certain loading stage, leading to
539 the fracture initiation. The details of this process were not clear and were frequently omitted
540 in the models by introducing the initial microcracks (seeds) with certain lengths and
541 orientations. Here we focus on these details and show for the first time that after initial elastic
542 loading, the competent elastoplastic layer sandwiched between incompetent (less brittle)
543 layers undergoes inelastic straining (damage) locally in the vicinity of the layer interfaces.
544 This damage is first distributed and then localizes into narrow pure dilation bands where it is
545 strongly accelerated and results in complete material failure and fracture initiation. Short
546 initial fractures corresponding to the narrow bands of failed material are normal to the least
547 local stress. They then propagate from the interfaces to the layer center with further extension,
548 which agrees with geological observations and experimental studies. Since deformation
549 localization is a bifurcation phenomenon, its numerical models are mesh-dependent and
550 require an enrichment to eliminate or reduce this dependence. This issue is the subject of a
551 careful study here with two regularization approaches. One is to ensure the same energy
552 dissipation within the deformation/fracture bands for different mesh sizes Δz (hence different
553 band widths in the models) by integrating Δz into the constitutive formulation. The classical
554 viscous regularization applied allows to avoid the ill-posedness of the initial boundary value
555 problem, although it has little effect on the results. The orientation of the deformation bands
556 and the resulting fractures is defined by the constitutive law and stress orientation. However,
557 in the numerical model it is also affected by the mesh geometry and notably by the grid lines.
558 This effect was strongly reduced using double brick-wedge grids. The proposed modeling
559 approach can be used for natural or induced fracture modeling in various contexts.

560

561 CRediT authorship contribution statement

562 Alexandre Chemenda: Conceptualization, Methodology, Software, Writing. Riad Hassani:
563 Methodology, Software, Writing - review & editing. Jinyang Fan: Investigation, Writing -
564 review & editing.

565

566 Declaration of Competing Interest

567 The authors declare that they have no known competing financial interests or personal
568 relationships that could have appeared to influence the work reported in this paper.

569

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574

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740 **Figure captions**

741 Figure 1. Field examples of layered and fractured sedimentary rocks. (a) Alternating
 742 incompetent (mudrocks) and fractured competent (limestone) layers in Lilstock Bay,
 743 Somerset, UK (rock hammer for scale) from Schöpfer et al. (2011). (b) Thick densely
 744 fractured Urgonian limestone layers; Cassis, Provence, SE France from Chemenda et al.
 745 (2021).

746 Figure 2. Setup of 3-layer models. (a) Series of alternating incompetent (pink) and competent
 747 (blue) layers. (b) An elementary (repeating) element of this series which corresponds to the
 748 complete three-layer modeling setup. (c) A half-symmetry modeling setup, with thicknesses
 749 of layers 1 and 2 being $T_1/2$ and $T/2$, respectively. V_x and V_z are the velocities applied in the
 750 corresponding directions to layers 1 and 3. V_x causes deformation and fracturing of layer 2
 751 and V_z is to maintain constant average vertical (lithostatic) stress at the horizontal model
 752 boundaries. The y -normal model boundaries are fixed in the y -direction. The layers are
 753 separated by cohesive-frictional interfaces. The models are pre-stressed in the y - and z -
 754 directions as indicated below. Layers 1 and 3 are purely elastic and layer 2 is elastoplastic.
 755 $T_1 = T_1 = 0.2$ m, $T = 1$ m, and $L = 0.6$ m.

756 Figure 3. Composite yield surface $\sigma_3(\sigma_1, \varepsilon^p)$. (1) Tensile failure. (2) Shear failure. (3) Post
 757 failure (after complete failure). (4) Shows a zero-level of σ_3 . The red point (circle)
 758 corresponds to the initial stresses $\sigma_1 = \sigma_{xx}^{ini}$ and $\sigma_3 = 0$ applied to the models.

759 Figure 4. Setup of one-layer models (a) and grid geometries used (b to d). (b and c) Brick- and
 760 wedge-shaped grids, respectively. (d) Double-layer sheet grid, with the attached brick and
 761 wedge-shaped grids. $T = 0.1$ m, and $L = 0.2$ m.

762 Figure 5. Group 1. Evolution of strain localization and fracture (stages/columns 1 to 5) in
 763 three models (a to c) differing only by the γ value: in (a), $\gamma = \infty$; in (b), $\gamma = 0.1$, and in (c),
 764 $\gamma = 0.01$. Deformation stages 1 to 5 correspond to ε_{xx} equal to -5×10^{-6} , -1.5×10^{-5} ,
 765 -6×10^{-5} , -4.5×10^{-4} , and -7.8×10^{-4} , respectively. $\Delta z = 5$ mm and $\varepsilon^0 = 0.02$. All the
 766 models have wedge-shaped grids shown in Fig. 4c.

767 Figure 6. Group 2. Impact of the grid geometry, resolution, and the regularization parameter γ
 768 on the dilation banding and structural stress-strain response. Final stages of strain localization
 769 and fracture are shown for five models with brick- (a) and wedge-shaped (b) meshes,
 770 respectively. The resolution of the models in columns 1 and 3 is $\Delta z = 5$ mm, in columns 2
 771 and 4, 2.5 mm, and in column 5, 1.25 mm. In columns 1 and 2, $\gamma = \infty$, and in columns 3 to 5,
 772 $\gamma = 1 \times 10^{-3}$. (c to h) Nominal stress-strain curves $\sigma_{xx}(\varepsilon_{xx})$ in the presented models. Since
 773 the models are pre-stressed to σ_{xx} close to $-\sigma_t^0$, the curves start near the initial failure (yield)
 774 point except in (c), where the elastic loading stage (segment) is added to the curves in (d). The
 775 curves in (d and e) are respectively for the models in columns 1 and 2 (curve (c) is for column
 776 1 as well). Curves in (g), are for the regularized brick-shaped models in (a3 to a5) with
 777 different resolutions indicated on the plot. (h) Curves for the regularized models with the
 778 brick, wedge, and double brick-wedge grids corresponding to the curves of different colors as
 779 indicated in (h). Solid curves are for $\Delta z = 1.25$ mm, and the dashed ones, for $\Delta z = 2.5$ mm.

780 Figure 7. Group 3. Final stages of strain localization and fracture in the models with brick (a),
 781 wedge (b), and double brick-wedge (c) grids. The columns 1 to 3 correspond to different
 782 orientations of the initial stress axes defined by angle ψ between σ_1 (shown by the white
 783 dashed lines) and the vertical; ψ is 0° , 15° , and 30° in columns 1, 2, and 3, correspondingly.
 784 In column 4, $\psi = 30^\circ$. The rotation of the initial stress axes is achieved by imposing the

785 corresponding normal and shear initial and boundary stresses. Models in columns 1 to 3 are
 786 inviscid ($\gamma = \infty$), and in column 4, $\gamma = 1 \times 10^{-3}$. In all models $\Delta z = 2.5$ mm and $\varepsilon^0 = 0.02$.

787 Figure 8. Group 4. (a to d) Final stages of strain localization and fracture in the inviscid
 788 models with double brick-wedge grids and different ε^0 and Δz related by Eq. (8): (a) $\varepsilon^0 =$
 789 0.01 and $\Delta z = 10$ mm; (b) $\varepsilon^0 = 0.02$ and $\Delta z = 5$ mm; (c) $\varepsilon^0 = 0.04$ and $\Delta z = 2.5$ mm; (d)
 790 $\varepsilon^0 = 0.08$ and $\Delta z = 1.25$ mm. (e) Nominal stress-strain curves from the models presented
 791 and other similar ones with different Δz (and hence ε^0): for (1) $\Delta z = 0.625$ mm; (2) $\Delta z =$
 792 1.25 mm; (3) $\Delta z = 2$ mm; (4) $\Delta z = 2.5$ mm; (5) $\Delta z = 2.7$ mm; (6) $\Delta z = 5$ mm; (7) $\Delta z = 10$
 793 mm. (f) Nominal stress-strain curves obtained from other models with $\Delta z = 1.25$ mm, $\varepsilon^0 =$
 794 0.08 , and different γ indicated on this figure.

795 Figure 9. Group 5. Four evolutionary stages (columns 1 to 4) of strain localization and
 796 fracture in five 3-layer inviscid models (lines a to e) with double brick-wedge grids for layer
 797 2; only this layer (its half, Fig. 2c) is shown. The models differ only by Δz and ε^0 ; in (a to c),
 798 they are related by Eq. (8): (a) $\Delta z = 1.25$ mm, $\varepsilon^0 = 0.08$; (b) $\Delta z = 2.5$ mm, $\varepsilon^0 = 0.04$; (c)
 799 $\Delta z = 5$ mm, $\varepsilon^0 = 0.02$. In (d), $\Delta z = 5$ mm, $\varepsilon^0 = 0.022$, and in (e), $\Delta z = 10$ mm, $\varepsilon^0 =$
 800 0.012 . The deformation stages shown (columns 1 to 4) correspond respectively to ε_{xx} of
 801 -6×10^{-4} , -9×10^{-4} , -2.1×10^{-3} , and -6×10^{-3} . (f) The stress-strain curves obtained
 802 from one-layer models for the same Δz and ε^0 as in the models a to e in this figure (the solid-
 803 line curves are the same as the corresponding curves in Fig. 8e).

804 Figure 10. Group 6. Four evolutionary stages (columns 1 to 4) of strain localization and
 805 fracture in three 3-layer models (lines a to c) with double brick-wedge grids for the shown
 806 layer 2. The models differ only in the γ value: it is ∞ , 0.15 , and 0.01 in (a, b, and c),
 807 respectively. In all models $\Delta z = 2.5$ mm, $\varepsilon^0 = 0.04$; the deformation stages (1 to 4)
 808 correspond to the same ε_{xx} values as in the previous figure (see caption of Fig. 9).

809 **Nomenclature**

810	E	Young's modulus
811	ν	Poisson's ratio
812	G	Shear modulus
813	K	Bulk modulus
814	ε^p	Accumulated inelastic (plastic) volume strain
815	$\sigma_t(\varepsilon^p)$	Tensile strength which is function of ε^p
816	σ_t^0	Initial (at $\varepsilon^p = 0$) tensile strength
817	$\sigma_c(\varepsilon^p)$	Unconfined (uniaxial) compression strength
818	σ_c^0	Initial value of σ_c
819	α_c, β_c	Material parameters in equations (1) and (4)
820	β_c^0	Initial value of β_c
821	σ_{ij}	Stress tensor, $i, j = 1, 2, 3$
822	ε_{ij}	Strain tensor
823	σ_i	Principal effective stresses, compression positive, $i = 1, 2, 3$
824	$\sigma_{int}(\varepsilon^p)$	Equal to the major stress σ_1 at the intersection of tensile and shear yield
825		envelopes in the (σ_1, σ_3) space (equation (2))
826	σ_{int}^0	Initial value of σ_{int}
827	β	Dilatancy factor (equation (6))
828	ε^0	Inelastic volume strain at which σ_t , σ_c , σ_{int} , and β reach zero
829	ρ	Density
830	k_n and k_s	Normal and shear stiffnesses of the interfaces
831	x, y, z	Axes defined in Fig. 2
832	$\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$	Horizontal and vertical (lithostatic) effective normal stresses

833	$\sigma_{xx}^{ini}, \sigma_{yy}^{ini}, \sigma_{zz}^{ini}$	Initial effective stresses in the numerical models
834	V_x and V_z	Rates applied to the model boundaries in the corresponding directions
835	τ^{int}	Shear stress along the interfaces between the layers
836	τ_0^{int}	Interface shear strength
837	c^{int}	Interface cohesion
838	μ^{int}	Interface friction coefficient
839	T_1, T_2 , and T	Thicknesses of the layers defined in Figure 2a
840	L	Length of the models
841	S	Fracture spacing
842	ψ	angle between σ_1 and the vertical
843	σ_{xx} and ε_{xx}	Nominal horizontal tension stresses and extension strains, respectively
844	F, F_t, F_s	Yield functions defined in equations (1)
845	Φ, Φ_t, Φ_s	Plastic potential functions defined in equations (4)
846	η	Relaxation time, equation (10)
847	γ	Regularization (viscous) parameter, equation (12)
848	Δz	Numerical grid element (zone) size
849	d_0	Thickness of the deformation or fracture band in numerical models
850	Δd	Change of the width of dilation bands during extension of the models
851	C, ε^0	Defined in equation (8)
852		