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Two sides of a fault: Grain-scale analysis of pore pressure control on fault slip

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The two sides of a fault: grain-scale analysis of pore pressure control on fault slip

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Pore fluid pressure in a fault zone can be altered by natural processes (e.g., mineral dehydration and thermal pressurization) and industrial operations involving subsurface fluid injection/extraction for the development of energy and water resources. However, the effect of pore pressure change on the stability and slip motion of a preexisting geologic fault remains poorly understood; yet it is critical for the assessment of seismic hazard. Here, we develop a micromechanical model to investigate the effect of pore pressure on fault slip behavior. The model couples fluid flow on the network of pores with mechanical deformation of the skeleton of solid grains. Pore fluid exerts pressure force onto the grains, the motion of which is solved using the discrete element method. We conceptualize the fault zone as a gouge layer sandwiched between two blocks. We study fault stability in the presence of a pressure discontinuity across the gouge layer, and compare it with the case of continuous (homogeneous) pore pressure. We focus on the onset of shear failure in the gouge layer, and reproduce conditions where the failure plane is parallel to the fault. We show that when the pressure is discontinuous across the fault, the onset of slip occurs on the side with the higher pore pressure, and that this onset is controlled by the maximum pressure on both sides of the fault. The results shed new light on the use of the effective stress principle and the Coulomb failure criterion in evaluating the stability of a complex fault zone. **PACS** numbers:

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I. INTRODUCTION

Geological faults form as a result of the failure of rock ⁵⁵ 28 in the Earth's crust, and slip along an existing fault can 56 29 generate hazardous earthquakes. It has long been known 57 30 that man-made fluid pressure changes due to factors such 58 31 as impoundment of reservoirs, surface and underground ⁵⁹ 32 mining, withdrawal of fluids and gas from the subsurface, ⁶⁰ 33 and injection of fluids into underground formations, are ⁶¹ 34 capable of reactivating pre-existing faults and thus induc-⁶² 35 ing earthquakes [1-5]. One of the well-known early ex-⁶³ 36 amples is the 1960s Denver Earthquake series, which was ⁶⁴ 37 induced by a deep waste fluid disposal well at the Rocky ⁶⁵ 38 Mountain Arsenal [1]. Not only can pore pressure be af-⁶⁶ 39 fected by anthropogenic processes, it can also be altered ⁶⁷ 40 in natural geologic systems. For example, earthquake 68 41 rupturing along a highly localized shear zone can gener-⁶⁹ 42 ate enough heat to cause local temperature rise and the 70 43 accompanying pore pressure increase due to expansion of ⁷¹ 44 pore fluid. This so-called thermal expansion process has ⁷² 45 been proposed as one of the key mechanisms to explain ⁷³ 46 dynamic fault weakening [6-8]. Despite the important 47 control pore pressure has on slip and faulting behavior, ⁷⁴ 48 the detailed dynamics and mechanisms involved in fault 75 49 reactivation remain poorly constrained [9, 10]. 50

Fault zones can have very complex internal structures,
 ⁷⁷ including the continuity of the fault rocks, the distribu-

tion and segmentation of slip surfaces, and the orientation, distribution and connectivity of subsidiary faults and fractures [11]. Flow and transport properties of fault zones can vary significantly from site to site, depending on the internal structure. A fault zone typically consists of two sub-structures: the fault core and the damage zone. The primary characteristic of fault cores is grain size reduction due to mechanical pulverization. The hydraulic properties of the fault core (gouge materials) can be very different from the fault damage zones and the undamaged host rock. Fault gouge is usually composed of fine particles/fragments. In many cases, the permeability of fault cores can be several orders of magnitude lower than that of a reservoir rock [12] and often acts as an impermeable boundary for fluid flow. In addition, hydraulic connectivity across the fault may be lost, for example, due to clay smearing or juxtaposition of a relatively high permeability reservoir rock with a low permeability rock from another formation [13]. Juxtaposition of two different rock types can also lead to difference in frictional strength on the two sides of a fault.

Numerical modeling of coupled flow and geomechanics is a valuable tool in assessing seismic hazard in large-scale reservoir systems. The effective stress principle together with the Mohr–Coulomb failure criterion has been applied in numerical modeling to explain fault reactivation due to fluid injection and to predict fault stability [see e.g., 14–19]. Reactivation of faults may occur if the shear stress on the fault exceeds the fault strength which is governed by the frictional properties and the effective normal

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stress. It is unclear, however, how conventional Mohr-141 83 Coulomb theory should be applied to the case where₁₄₂ 84 there is a substantial pressure difference across the fault₁₄₃ 85 zone due to fault cores that are considered impermeable144 86 over the time scale of interest. In their coupled mul-145 87 tiphase flow and geomechanics model, Jha and Juanes146 88 [17] proposed to calculate the fault pressure in the failure147 89 criterion to be the maximum of pressures on both sides of₁₄₈ 90 the fault, which is represented by a 2D interface element₁₄₉ 91 in a 3D mesh. If the fault pressure is taken as the arith- $\scriptstyle\rm 150$ 92 metic average across the fault or is obtained from volume₁₅₁ 93 element based pressure, a coupled modeling analysis may₁₅₂ 94 predict a higher fault strength at any given time and re-153 95 sult in a delayed onset of fault reactivation (than that 96 with the maximum pressure), which, consequently, can 97 lead to erroneous estimations of maximum fluid injection 98 rate/volume in practical situations. Therefore, it is criti-99 cal to carefully examine the role of pressure discontinuity 100 in controlling fault stability. 101

Theoretical studies based on the continuum approach 102 [see e.g., 20, 21] have addressed the issue of pore pres- $_{\scriptscriptstyle 155}$ 103 sure discontinuity due to existence of material with dif-104 ferent hydraulic parameters across the fault. Considering 105 a spontaneously propagating rupture along an interface₁₅₈ 106 between dissimilar poroelastic materials, these studies 107 have provided important insights on how pore $\operatorname{pressure}_{160}^{10}$ 108 change induced by an imposed fast slip between dissim- $^{100}_{161}$ ilar poroelastic materials can influence the stability of $^{161}_{162}$ 109 110 earthquake ruptures. In addressing the important issue $_{163}$ 111 of fault dynamic weakening by flash heating and thermal 112 pressurization, Rice [7] ruled out the possibility that $\frac{1}{165}$ 113 shear deformation in the gouge is distributed across the $_{166}$ 114 gouge during dynamic earthquake slip. 115 167

Fault gouge can be considered a dense granular mate-168 116 rial whose deformation is controlled by the collective mo-169 117 tion of the constituent particles. Continuum models of_{170} 118 deforming granular material rely on constitutive laws in₁₇₁ 119 which the formulation of continuum deformation requires₁₇₂ 120 a projection scheme to relate the continuum deformation₁₇₃ 121 to the underlying motion of the grains [22]. In contrast, $_{174}$ 122 models based on the discrete element method $(DEM)_{175}$ 123 treat individual particles explicitly, and have effectively $_{176}$ 124 captured emergent phenomena, such as shearing band-177 125 ing and stick-slip in deforming granular materials [see₁₇₈ 126 e.g., 22–30]. In this study, we adopt a DEM framework, 179 127 and instead of imposing slip, we simulate emergence of_{180} 128 slip around a fault gouge layer with two interfaces with₁₈₁ 129 the bounding material. Numerical simulations—mostly₁₈₂ 130 based on DEM [e.g., 25-27, 29, 31, 32]—have been used₁₈₃ 131 132 to understand the fundamental role gouge material plays₁₈₄ in determining fault frictional properties and strength.₁₈₅ 133 These previous numerical studies on faulting or shear-186 134 ing, however, have not considered the effect of pore fluid₁₈₇ 135 pressure coupling. We present evidence, based on a grain-188 136 scale analysis, in support of the choice of using the max- $_{189}$ 137 imum fluid pressure across the fault for evaluation of the $_{190}$ 138 failure criterion. 139 191

¹⁴⁰ In short, accurate prediction of fault stability requires¹⁹²

detailed understanding of the role of pore pressure. In this work, we develop a micromechanical model at the grain scale and perform one-way coupled simulations to investigate the effect of pore pressure on fault slip behavior. We consider a block–gouge system where the block represents the fault walls. We study fault stability in the presence of a pressure discontinuity across the gouge layer, and compare it with cases of homogeneous pore pressures. We focus on the onset of shear failure along the block–gouge interfaces, and provide new insights on the use of the effective stress principle and the Coulomb failure criterion in evaluating the stability of a complex fault zone.

II. METHODS

We develop a three-dimensional micromechanical model, which is based on the discrete element method (DEM) coupled with a pore network flow (PNF) model, illustrated in Fig. 1. In the DEM, the solid phase is represented by spherical grains and contact interaction among them. The spatial arrangement of grains forms an interconnected void space, from which a pore network, comprised of pore bodies and pore throats, is extracted through tetrahedral (weighted Delaunay) tessellation of grain centroids (see Fig. 1(a)-(b)). The pore body volumes and the pore throat conductances are calculated based on the void space geometry. The fluid in the pore network interacts with the solid grains, giving rise to hydro-geomechanical coupling. On the one hand, the pore fluid exerts pressure forces onto the grains, resulting in modified force balance and motion of the grains as compared to that in the dry system. On the other hand, deformation of the solid phase through rearrangement of the grains can also change the pore pressure and the pore-network topology. Our model updates the tetrahedral tessellation, and hence the pore-network (including its pore volumes and pore throat conductances), regularly during a simulation. The frequency of this updating procedure can be preset according to the timestep size or a certain threshold displacement of the grains. The PNF model solves the pressure evolution based on Darcian flow in the pore network and calculates the pressure forces onto the solid particles. Compared with other DEM-based poromechanical coupling approaches, including microscale models where fluid pressure is resolved below the pore scale [e.g., 33–35] and continuum-scale models in which flow is solved on a coarse grid at the scale of multiple grains [e.g., 36], the PNF approach [37–39] is advantageous in that it avoids the high computational cost in the microscale models and the inability to accurately describe the fluid-solid interaction at the particle scale in the continuum-scale models. Below, we describe the numerical model in detail.



FIG. 1. Schematic of the coupled hydromechanical model based on the Discrete Element Method (DEM) and a Pore Network Flow (PNF) model. (a) pore network in a five-grain setup (transparent yellow spheres); the pores are shown by purple spheres and the throat by a green cylinder; the edges of the tetrahedral tessellation are shown with red lines. Each pore is composed of the void space within a tetrahedron whose four nodes are the centers of the surrounding grains. Each throat is defined by the open area within a triangular face of a tetrahedron. The pore volumes and throat conductances are calculated based on local geometry. (b) grain pack (cut in half and rendered in 50% opaque yellow color) and accompanying pore network. (c) schematic of the couplings in the DEM–PNF model.

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Α.

Discrete element method

Our three-dimensional (3D) micromechanical model²¹² 194 couples the discrete element method (DEM) and a pore- $^{\scriptscriptstyle 213}$ 195 network fluid flow model. The modeling concept is based 196 on the idea of two interacting, overlapping networks: one²¹⁴ 197 for the solid matrix and the other for the pore fluid 198 [37, 38]. In DEM, spherical grains are numerically gener-199 ated and the mechanics of the grain motions are solved.²¹⁵ 200 The translational motion of each grain in the system is²¹⁶ 201 governed by Newton's second law: 202 218

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$$m_i \ddot{\mathbf{x}}_i = \sum_j \mathbf{F}_j^c + \sum_k \mathbf{F}_k^p,$$
 $(1)_{220}^{216}$

where m_i is the mass of *i*th grain whose position vector is \mathbf{x}_{i} , \mathbf{F}_{j}^{c} is the force applied on contact *j* of the grain, and \mathbf{F}_{k}^{p} is the pressure force applied by *k*th pore surrounding₂₂₅ the grain. The pressure force on *i*th grain by *k*th pore is calculated by:

$$\mathbf{F}_{k}^{\mathrm{p}} = \int_{\partial \Gamma_{k}^{i}} p_{k} \mathbf{n} \,\mathrm{d}s, \qquad (2)^{229}_{230}$$

where $\partial \Gamma_k^i$ is the fluid-solid interface for *i*th grain and *k*th pore (with pore pressure p_k), **n** is the unit vector pointing from the centroid of the pore to the centroid of the grain. The rotational motion of each grain is described by:

$$\mathbf{I}_i \ddot{\boldsymbol{\theta}}_i = \sum_j \mathbf{M}_j^{\mathrm{c}},\tag{3}$$

where \mathbf{I}_i is the tensor of moments of inertia of grain iwith the vector of rotation angles $\boldsymbol{\theta}_i$ around its centroid, and \mathbf{M}_j^c is the moment acting on grain i through contact j. The pressure force points from the centroid of a pore to the centroid of a grain; it does not induce moments on grains. We use the PFC3D code [40] to solve the equations of motion simultaneously for all grains in the system and to integrate these equation in time.

While fluid pressure influences grain motions through the application of pressure forces, the movement of grains deforms the individual pores, thus altering the pore pressure distribution. At the same time, the pore pressure evolution is subject to Darcian flow under the prevailing hydrodynamic conditions. To solve the fluid pressure with the above interactions taken into account, we develop a 3D numerical model for pore-network flow (illustrated with Fig. 1 and Fig. 2), which is coupled to₂₇₆
PFC3D. This model is described in detail below. 277

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B. Pore network flow model

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As a discretization of the pore space, a pore network tis extracted from each numerically generated granular pack (see Fig. 1). We perform a 3D weighted Delaunay triangulation in which each vertex is the centroid of a grain and each tetrahedron contains a pore (Fig. 2).

Using basic geometry, we calculate the volume of each²⁶⁴ pore V_i by subtracting the volume of the solid part $V_i^{s^{265}}$ from the volume of a tetrahedron V_i^{tet} :

$$V_i = V_i^{\text{tet}} - V_i^{\text{s}}.$$
 (4)

²⁴³ The volume of the solid part $V_i^{\rm s}$ is calculated as:

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$$V_i^{\rm s} = \sum_{j=1}^4 V_j^{\rm sc} - \sum_{k=1}^6 V_k^{\rm so}, \tag{5}^{289}_{291}$$

where $V_i^{\rm sc}$ is the volume of the spherical cone of 293 245 each grain j (j = 1,2,3,4) inside the tetrahedron, and²⁹⁴ 246 $\sum_{k=1}^{6} V_k^{\text{so}}$ is the total solid overlap volume of the six pos-247 sible grain-grain contacts. Note that we do not consider 248 the overlap volume shared by more than two spheres be- $^{\scriptscriptstyle 295}$ 249 cause this overlap scenario does not occur in our sim-250 ulations owing to the fact that only very small $\operatorname{overlap}_{296}$ 251 distances are induced by realistic external forces. The₂₀₇ 252 pore throat length l_{ij} is taken as the distance between₂₀₈ 253 the centroids of tetrahedron i and tetrahedron j. The₂₉₉ 254 pore throat conductance C_{ij} is calculated based on the₃₀₀ 255 minimum cross-sectional area A_{ij}^{pt} on a triangular face be-₃₀₁ 256 tween tetrahedron i and j, the perimeter P_{ij}^{pt} associated 257 with A_{ij}^{pt} , and the fluid viscosity η as [38, 41]: 258 302

$$C_{ij} = \frac{3A_{ij}^{\text{pt}^3}}{5\eta P_{ij}^{\text{pt}^2}}.$$
 (6)³⁰³₃₀₄

The pore volumes, throat conductances, and throat³⁰⁶ lengths are all functions of the grain positions and radii,³⁰⁷ and are thus subject to change when the solid phase de-³⁰⁸ forms. In our model, we update these parameters on a₃₀₉ regular basis at a selected time interval.

When local accumulated grain displacement becomes³¹⁰ 265 large, i.e., comparable to the grain radius, the initial tri-311 266 angulation may no longer faithfully represent the pore 267 space constrained by the new grain positions. For exam-268 ple, this occurs when one grain slips past another. Using 269 the initial triangulation for pressure solution and force $^{\rm 312}$ 270 calculations may bring a source of error. In order to 271 minimize the potential error from the deteriorated rep-272 resentation of the pore space by the pore network due³¹³ 273 to large local deformation, we update the triangulation 274 regularly during a simulation. 314 275

Fluid mass balance over an pore V_i gives the following equation:

$$\frac{\delta V_i}{\delta t} + V_i^{\rm w} \beta_f \frac{\delta p_i}{\delta t} = -\sum_j q_{ij},\tag{7}$$

where δV_i and δp_i are the pore volume change (due to matrix deformation) and the pore pressure change after a time step δt , respectively, V_i^{w} is the volume of fluid in pore i ($V_i^{w} = \delta V_i$ in the case of pore network), β_w is the compressibility of the fluid and q_{ij} is the flux out of the pore domain to pore j through pore throat (i, j). The flux q_{ij} is calculated as:

$$q_{ij} = C_{ij} \frac{p_i - p_j}{l_{ij}}.$$
(8)

In Eq. (7), the two terms on the left hand side are analogous to the storage term in the diffusion equation of compressible flow in porous media. The pore pressure solution of Eq. (7) with Eq. (8) plugged in can be obtained by using two approaches. The first is an explicit scheme [38] with the fluxes calculated using pressure gradients from the last time step, giving the following equation to update fluid pressure in each pore:

$$\delta p_i = \frac{1}{\beta_w V_i} \left(-\delta V_i - \sum_j q_{ij} \delta t \right). \tag{9}$$

Note that numerical stability of the explicit pressure solution [Eq. (9)] imposes a timestep limit, and thus the timestep should be carefully chosen in a numerical simulation.

In this study, we propose the second approach, which employs an implicit finite-volume scheme:

$$\frac{\delta V_i}{\delta t} + V_i \beta_w \frac{p_i^{n+1} - p_i^n}{\delta t} = -\sum_j C_{ij} \frac{p_i^{n+1} - p_j^{n+1}}{l_{ij}}, \quad (10)$$

where the superscripts n and n + 1 represent the current timestep and the timestep to be advanced, respectively. The implicit scheme enjoys unconditional stability in terms of timestepping. Writing Eq. (10) for all pores results in a system of linear equations for pore pressure in matrix form:

$$\mathbf{\Lambda p^{n+1}} = \mathbf{b},\tag{11}$$

with entries $\lambda_{i,j}$ in Λ and b_i in **b** calculated, respectively, by:

$$\lambda_{i,j} = \begin{cases} \frac{V_i \beta_w}{\delta t} + \sum_{k=1}^4 \frac{C_{ik}}{l_{ik}} & \text{if } i = j \\ \\ -\frac{C_{ij}}{l_{ij}} & \text{if } i \neq j \end{cases}$$
(12)

and

$$b^{i} = -\frac{\delta V_{i}}{\delta t} + \frac{V_{i}\beta_{w}p_{i}^{n}}{\delta t} .$$
(13)



FIG. 2. Illustration of triangulation, pore network, and pore throat. (a) pore network in a five-grain setup; the pores are shown by purple spheres and the throat by a green cylinder; the edges of the tetrahedral tessellation are shown in red. Each pore is composed of the void space within a tetrahedron whose four nodes are the centers of the surrounding grains. The two pores have volumes V_i and V_j , and pressures p_i and p_j . Each pore throat having conductance C_{ij} and length l_{ij} is defined as the connection between two neighboring pores $(V_i \text{ and } V_j)$ through the void space. (b) The pore throat conductance C_{ij} is calculated based on the minimum cross-sectional area A_{ij}^{pt} on a triangular face between tetrahedron *i* and *j* (the shaded area), and the perimeter P_{ij}^{pt} associated with A_{ij}^{pt} .

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Pressure solutions obtained using the explicit and the³⁴³ implicit schemes take into account both the pressure diffusion and the effect of deformation of the solid matrix obtained from DEM. Thus, this fluid flow formulation³⁴⁴ coupled with the DEM framework captures the two-way³⁴⁵ budro mechanical coupling under sincle phase flow.

320 hydro-mechanical coupling under single-phase flow.

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C. Contact behavior

Two rheological models for contact behavior are used $^{\scriptscriptstyle 352}$ 322 in this study. The first is a linear elastic–frictional con-³⁵³ 323 tact law described in more detail in Cundall and Strack³⁵⁴ 324 [42]; this contact model is used for contacts on $\mathrm{gouge}^{^{355}}$ 325 particles. In this contact model, the contact force is pro-326 duced by linear springs with constant normal and shear^{357} 327 stiffnesses, $k_{\rm c}^{\rm n}$ and $k_{\rm c}^{\rm s}$. The linear springs cannot sustain³⁵⁸ 328 tension—the contact law is deactivated when the surface³⁵⁹ 329 gap $g_{\rm s}$ > 0, and slip is accommodated by imposing a³⁶⁰ 330 Coulomb limit on the tangential force using a constant³⁶¹ 331 friction coefficient μ . The second, which is used for con-362 332 tacts between the block particles, is the linear contact₃₆₃ 333 bond model described in more detail in Potyondy and₃₆₄ 334 Cundall [43]. This contact rheology provides the behav-365 335 ior of a linear elastic and either bonded or frictional in-366 336 terface that carries a force. The interface does not resist₃₆₇ 337 relative rotation and is either bonded or unbonded. If₃₆₈ 338 bonded, the behavior is linear elastic until the strength₃₆₉ 339 limit is exceeded and the bond breaks, making the in-370 340 terface unbonded. If unbonded, the behavior is linear₃₇₁ 341 elastic-frictional—equivalent to the first contact model. 372 342

D. Block-gouge system

Gouge materials play an important role in earthquake nucleation. They have been extensively studied experimentally [e.g., 10, 44–49], often with the primary interest of examining their frictional properties and slip instability characterized by the rate and state friction laws [50, 51]. A recent experimental study [49] reported that increasing pore-fluid pressure leads to a decrease in the internal friction coefficient of carbonate gouge sample, but the mechanisms behind this observation remain unexplained. Geller et al. [52] developed a 2D experimental setup of a plate-granular rods system under dry condition, and analyzed the stick-slip dynamics of the granular layer undergoing shear using digital image analysis. Despite recent advances in 3D experimental techniques in measuring forces at the grain scale [53, 54], real time imaging of grain displacement and forces remains challenging for granular packs in dynamic deformation.

Here, we apply the coupled DEM–PNF model described above to a representation of a fault zone consisting of a gouge layer sandwiched between two blocks; the block material is represented by a group of contactbonded particles and the gouge is composed of unbonded particles (Fig. 3). Note that we invoke the one-way coupled assumption here (see Discussion section). (A similar scenario is also considered where the fault normal is aligned with the principal stress axis of σ_{xx} and where a periodic boundary condition is used in the z direction; see Supplementary Material [55].) For the gouge particles, the contact behavior between particles follows an

elastic-frictional contact law [42]. For the blocks, con-424 373 tact bonds are assigned to the particles. Once the tensile425 374 and shear strengths of a bond are exceeded, the bond₄₂₆ 375 breaks and the contact between the originally bonded₄₂₇ 376 pair of particles is described by the elastic-frictional con-428 377 tact law. To generate the block-gouge assembly, we first₄₂₉ 378 generate an isotropic initial packing under static equilib-430 379 rium, following a widely adopted procedure [43]. Contact₄₃₁ 380 bonds are then included and boundary walls are used to₄₃₂ 381 apply an initial stress to the pack. 433 382

383 E. Boundary conditions and system parameters 436

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The boundary conditions are shown in Fig. 3. To initi-384 ate macroscopic fault slip, we apply load in the horizontal⁴³⁷ 385 (x) direction using the left and right rigid walls with a 386 constant strain rate ($\dot{\varepsilon}_h = \frac{\Delta x}{L_x \Delta t} = 7.8 \times 10^{-3} \text{ s}^{-1}$). We₄₃₈ keep track of the horizontal stress σ_h at the left and right₄₃₉ 387 388 wall boundaries. A zero displacement boundary is im-440 389 posed for faces in the out-of-plane (y) direction $(u_y = 0)_{.441}$ 390 On the top and bottom faces of the blocks, we use a_{442} 391 servo-controlled vertical stress σ_v of 1.0×10^7 Pa. We₄₄₃ 392 are interested in reproducing relative slip between the₄₄₄ 393 two blocks that minimizes finite-size effects, that is, slip₄₄₅ 394 along a plane that is parallel to the fault. To this end_{446} 395 we impose zero-displacement boundary conditions in the₄₄₇ 396 vertical (z) direction at the gouge layer ($u_z^g = 0$). To₄₄₈ 397 investigate the effect of pore pressure, we consider five₄₄₉ 398 different cases of pore-pressure distribution (Fig. 3). We_{450} 399 slowly increase the pore pressure from zero to a prede-451 400 termined final pressure ($p_t = 2.5 \times 10^7$ Pa for Case 1_{452} 401 and $0.5p_t = 1.25 \times 10^7$ for Case 4). Cases 2 and 3 are₄₅₃ 402 designed such that at all times, they have the same max-403 imum pore pressure in the gouge as in Case 1 and have 404

the same average pore pressure as in Case 4.

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406 Case 1	The pore pressure increases uniformly (from 0 at
407	zero horizontal strain) on both sides of the gouge ⁴⁵⁵
408	layer to the final value $(p^L = p^R = p_t)$ at horizontal ⁴⁵⁶
409	strain of 3.1×10^{-3} , where p^L and p^R are the pore ⁴⁵⁷
410	pressures on the left and right blocks, respectively. ⁴⁵⁸

⁴¹¹ Case 2 The pore pressure increases (from 0 at zero horizon-⁴⁶⁰ ⁴¹² tal strain) on the left side of the gouge layer until⁴⁶¹ ⁴¹³ $p^L = p_t$ at horizontal strain of 3.1×10^{-3} , while the⁴⁶² ⁴¹⁴ pressure on the right side is held constant at zero⁴⁶³ ⁴¹⁵ value, $p^R = 0$. A linear gradient across the fault is⁴⁶⁴ ⁴¹⁶ maintained. ⁴⁶⁵

⁴¹⁷ Case 3 Reverse of Case 2, with $p^L = 0$ and p^R increases to ⁴¹⁸ p_t .

⁴¹⁹ Case 4 Homogeneous pressure evolution, but only up to ⁴²⁰ half the value of Case 1, $p^L = p^R = 0.5p_t$.

- ⁴²¹ Case 5 Homogeneous pressure corresponding to the dry⁴⁷² ⁴²² system with zero pore pressure, $p^L = p^R = 0$.
- ⁴²³ The simulation parameters are listed in Table I.

Even though our grain-scale coupled model captures the two-way coupling between flow and mechanical deformation, it is beneficial, from a standpoint of computational efficiency, to consider the assumption of one-way fluid to solid coupling in a given situation. Two-way coupling requires that pore geometry and throat conductance are updated at each time step, which is computationally intensive. Comparison of simulation results between the one-way and two-way coupling models justifies the simplifying assumption of one-way coupling (see discussions in Sec. IV). Thus, in the rest of our simulations we invoke this simplifying assumption and prescribe the pore pressure without solving for its evolution.

III. RESULTS

In this section, we present numerical results for the five cases of pore pressure distribution. Our model setup resembles a triaxial configuration of a gouge laver friction experiment with pore pressure control. The gouge layer failure is driven by mechanical loading on the blocks. In the model, the grain rearrangement by rotation and intergranular slip is responsible for deformation of the gouge layer. Our focus is on the onset of shear failure under different pressure controls with special attention to cases where a discontinuity in pressure across the gouge layer exists, $p^L \neq p^R$. The fault normal stress σ_n is calculated as $\sigma_n = \frac{1}{2}(\sigma_h + \sigma_v) + \frac{1}{2}(\sigma_h - \sigma_v) \cos 2\alpha$, where α is the angle of the gouge layer with respect to the horizontal and σ_h and σ_v . For a more intuitive interpretation of the results, we follow the convention that compressive stresses are positive.

A. Grain displacement and contact forces

Snapshots of grain displacement during the fault failure are presented in Fig. 4. These snapshots are taken at the same time point corresponding to a horizontal strain of $\varepsilon_h = 3.1 \times 10^{-3}$. It is evident from these snapshots that the spatial distribution of pore pressure strongly influences the deformation. For example, when the pore pressure is continuous across the fault (Case 1, Fig. 4(a)), the displacement pattern is largely symmetric, with the foot wall moving down, and the hanging wall moving up as a result of the imposed reverse faulting conditions. The slip of blocks initiates along the two gouge-block interfaces. At late times, strain localization is evident as the slip surfaces gradually shift towards the center of the gouge layer [56]. The faulting behavior is markedly different when the pressure is discontinuous across the fault(Cases 2-3, Fig. 4(c), (e)), accommodated with a strong pressure gradient within the gouge layer. For example, when $p^R > p^L$, the displacement of the hanging wall is significantly larger than that of the foot wall (Case 3, Fig. 4(e)). Moreover, slip is localized at the hanging-wall gouge-block interface, which is associated



FIG. 3. (a), 3D block–gouge system composed of 7878 particles. The light green particles are unbonded, representing the gouge, while the blue particles are bonded, representing the blocks (fault walls). The origin of axes is placed at the center of the gouge layer. Rigid frictionless walls (not shown) are used to provide mechanical boundary conditions. Loading in the x direction with constant velocity drives the system to slip failure. The front and back walls are assigned zero displacement condition ($u_y = 0$). To reproduce relative motion with respect to the gouge layer, we impose zero vertical displacement at the top and bottom of the gouge layer ($u_z^2 = 0$). (b), Pore pressure cases. Cases 1, 4 and 5 represent continuous pressure across the fault, with Case 4 having a pressure half of that in Case 1, and Case 5 having zero pore pressure (dry system). Cases 2 and 3 represent discontinuous pressure across the fault, with a strong pressure gradient within the gouge layer.

TABLE I. Simulation parameters.

Parameters	Value
Average grain diameter \overline{d}	0.002 m
min. and max. grain diameter d_{\min} , d_{\max}	0.0018, 0.0022 m
Grain-grain friction coefficient μ_{g-g}	0.5
Packing porosity ϕ	0.35
Contact normal stiffness k_n^c	$5.0 \times 10^{10} \text{ N/m}$
Contact shear stiffness k_s^c	$2.5 \times 10^{10} \text{ N/m}$
Contact bond tensile strength T , (mean \pm std)	$(1.0 \pm 0.2) \times 10^9$ Pa
Contact bond shear strength S , (mean \pm std)	$(1.0 \pm 0.2) \times 10^9$ Pa
Gouge layer width w	0.012 m
Gouge layer dip angle α	45°
Maximum pore pressure (p_t)	2.5×10^7 Pa
Domain size L_x, L_y, L_z	0.08, 0.02, 0.05 m



FIG. 4. Slip behavior for the block–gouge system. Particle displacement in the z direction (left column) and contact force network with both color and link size representing force magnitude (right column) at horizontal strain $\varepsilon_h = 3.1 \times 10^{-3}$. (a)–(b): pore pressure Case 1; (c)–(d): Case 2; (e)–(f): Case 3; (g)–(h): Case 4; (i)–(j): Case 5.

ment of the two blocks.

 $_{476}$ $\,$ with the higher pore pressure. In Case 4 where the pore $_{481}$

 $_{477}$ $\,\,$ pressure is half of that in Case 1, we observe a significant

 $_{478}$ decrease of the magnitude of grain displacement in the 482

 $_{479}$ z direction. The simulation with dry condition (Case 5, 483 $_{480}$ Fig. 4(i)) produces the smallest relative vertical move- 484

Contact force networks corresponding to the grain displacement snapshots discussed above are shown in the right column of Fig. 4. Pore fluid exerts pressure forces on the particles, which reduces the contact forces, with



FIG. 5. Histogram of normal component of contact forces in the gouge layer for the scenario considered in the main text. (a) pore pressure case 1; (b) pore pressure case 3.

a macroscopic consequence of effective stress. The con-520 486 tact forces in the blocks are strongly influenced by the₅₂₁ 487 pore pressure distribution. When the pore pressure is522 488 uniform in the block-gouge-block system (Fig. 4(b), (h),⁵²³ 489 (j)), the results show that the contact force network ex-490 hibits no overall difference between the left and right₅₂₄ 491 blocks. In contrast, for the inhomogeneous pore pressure₅₂₅ 492 cases (Fig. 4(d),(f)), the difference in the contact force₅₂₆ 493 network between the left and right blocks is apparent. 527 494 The horizontal loading initially compacts the gouge⁵²⁸ 495 layer, which causes a rapid increase in the magnitude of⁵²⁹ 496 contact forces [56]. The fabric of the contact force net-530 497 work evolves and chains of strong contact forces develop⁵³¹ 498 across the gouge layer as a result of loading. The con-532 499 tact force chains in the gouge layer are oriented roughly⁵³³ 500 parallel to the loading direction and are distributed more⁵³⁴ 501 or less evenly along the gouge layer (Fig. 4), indicating⁵³⁵ 502 that the results are not strongly affected by finite-size⁵³⁶ 503 effects. The number of contacts in the gouge layer drops⁵³⁷ 504 by about 20%, and the maximum contact force magni-538 505 tude increases by about an order of magnitude with only⁵³⁹ 506 small differences between pore pressure cases (Fig. 5). 540 507 541

⁵⁰⁸ B. Evaluation of equivalent fault pressure p^{f}

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The transition from gouge layer compaction to slip is545 509 characterized by a sharp increase in vertical strain rate546 510 $\dot{\varepsilon}_v$ in all pore pressure cases (Fig. 6(a)). Here, $\dot{\varepsilon}_v$ is de-547 511 fined as the difference in vertical velocity between the548 512 top of the hanging wall block and the bottom of the foot549 513 wall block, divided by L_z . Before slipping, the horizontal⁵⁵⁰ 514 stress builds up rapidly, and the blocks dilate vertically, 551 515 which characterizes the initial vertical strain rate as the⁵⁵² 516 gouge layer compacts. Comparison of cases 1, 4, and 5553 517 (Fig. 6(a)) reveals that, when the pore pressure is lower, 554 518 the onset of slip occurs at a later time and, hence, at a555 519

larger normal stress due to larger loading strain accumulated. In our scenario, the delayed onset of slip causes additional compaction of the gouge layer (as a result of horizontal loading), which strengthens the material.

One of our main interests is to see how the fault pressure should be evaluated in the block-gouge-block system with a pore pressure contrast between the two blocks. From Fig. 4 we observe that when there is a pore pressure difference across the fault, the onset of slip appears to be controlled by the *maximum* of pore pressure on either side of the gouge layer, $\max(p^L, p^R)$. Indeed, Fig. 6 also shows that the strain rate-stress curves for Cases 1, 2 and 3 turn sharply around the same normal stress and effective normal stress values, while Case 4 exhibits a much delayed turning point. Note that $\max(p^L, p^R)$ is identical for Cases 1, 2 and 3, while $(p^L + p^R)/2$ is the same for Cases 2, 3 and 4. Our result suggests that the onset of failure for Cases 2 and 3 behaves similarly to that for Case 1 rather than Case 4. This result indicates that in the effective stress principle $\sigma_n^{\text{eff}} = \sigma_n - p^f$, the fault pressure p^f should be evaluated using the maximum of pore pressure on both sides instead of using the average.

In an additional scenario [55] where the fault normal is aligned with the direction of the principal stress σ_{xx} , the results confirm that the slip favors the side of the fault with a higher pore pressure when there is a substantial difference in pore pressure (Cases 2–3) between the two sides [55]. More importantly, by evaluating whether the system fails by slip or not, we can clearly distinguish Cases 2–3 from Case 4. Note that the arithmetic average of pore pressure in the fault gouge layer in Cases 2–3 equals to that in Case 4. This result further demonstrates the point that by assigning the arithmetic average of pressure to the situation where there is a strong pressure change across the fault one can make incorrect predictions of fault stability.



FIG. 6. (a) Vertical strain rate $[s^{-1}]$ as a function of normal stress in the fault gouge. (b) Vertical strain rate $[s^{-1}]$ as a function of *effective* normal stress $\sigma_n^{\text{eff}} = \sigma_n - p^f$ with fault pressure $p^f = \max(p^L, p^R)$.

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IV. DISCUSSION

In the simulations shown above, for computational effi-557 ciency we have made the simplification of assuming one-558 way fluid to solid coupling. The one-way coupling scheme 559 here implies that the influence of solid matrix deforma-560 tion on pore pressure is neglected, i.e., the first term on 561 the left hand side of Eq. (7) is dropped. To test the 599 562 validity of the assumption in our case of slip along $a^{\scriptscriptstyle 600}$ 563 block-gouge interface, we have simulated fault slip us-601 564 ing both the one-way and the two-way coupling methods 602 565 (see Fig. 7). In both cases, a homogeneous initial pore 603 566 pressure $p_0 = 0$ is assigned in the pack. The pore pres-567 sure evolution is traced in the two-way coupling case.⁶⁰⁵ 568 The results show that the difference in grain displace-606 569 ment between the two simulations are indeed negligible⁶⁰⁷ 570 (Fig. 7(b)-(c)). The slip between the block and the gouge 571 reduces pore pressure along the shearing zone due to dila-572 tion (Fig. 7(d)), but the maximum pressure change due_{608} 573 to mechanical shear (induced by loading on top of the 574 block) is less than 1 kPa, almost four orders of magni-575 tude smaller than the horizontal stress component. 576 610

To further substantiate that a one-way coupled ap-611 577 proach is a good approximation in our problem setup,₆₁₂ 578 we compare two time scales in the system, the fluid pres-613 579 sure relaxation time scale $t_p,$ and the pore deformation $_{\tt 614}$ 580 time scale t_d . The time scale t_p can be calculated as₆₁₅ 581 $(L_x/2)^2/D_h$, where L_x is the domain size in the horizon-⁶¹⁶ 582 tal direction and D_h is the hydraulic diffusivity $k_0/(\beta_w \eta)^{_{617}}$ 583 with k_0 being the mean permeability (which can be es-618) 584 timated by running a Darcy flow simulation with pre-619 585 scribed pressure gradient), and β_w and η the compress- $^{\rm 620}$ 586 ibility and viscosity of water, respectively. The time scale⁶²¹ 587 t_d is approximated as d_p/v , where d_p is a representative⁶²² 588 pore diameter (which is taken as 0.1d) and v is a load-623 589 ing velocity. Substituting parameter values considered in₆₂₄ 590 this study, $L_x/2 = 2.0 \times 10^{-2}$ m, $k_0 = 1.0 \times 10^{-9}$ m²,₆₂₅ 591

 $\beta_w = 4.5 \times 10^{-10} \text{ Pa}^{-1}$, $\eta = 1.0 \times 10^{-3} \text{ Pa} \cdot \text{s}$, and $v = 1.0 \times 10^{-2} \text{ m/s}$, we obtain t_p on the order of 10^{-8} s, and t_d on the order of 10^{-2} s. The separation of time scales in this system means that pore pressure will not change significantly due to fast dissipation through the pore space. This calculation justifies the one-way coupling assumption.

It should be pointed out that grain fragmentation, which can occur in a physical experiment involving pulverization, is not taken into account due to computational constraints. Grain size reduction during shear of fault gouge has been numerically studied using DEM under dry conditions, i.e., when the hydraulic coupling is not considered [32, 57]. The effect of fluid pressure on evolution of shearing fault gouge remains to be investigated in future studies.

V. CONCLUSIONS

In summary, we have developed a 3D micromechanical model that couples a pore network flow (PNF) model to a discrete element model (DEM). The model couples fluid flow on the network of pores with mechanical deformation of the skeleton of solid grains. Pore fluid exerts pressure force onto the grains, the motion of which is solved using DEM. We have investigated the role of pore fluid pressure on slip failure of a block–gouge system. The fault zone is conceptualized as a gouge layer sandwiched between two blocks. Motivated by the problem of representing the fault pressure in the case of low across-fault permeability, we have studied the fault stability in the presence of a pressure discontinuity across the gouge layer, and compared it with the case of continuous (homogeneous) pore pressure.

Our micromechanical modeling results demonstrate the role of pore pressure in reducing the effective normal



FIG. 7. Comparison of slip along a block–gouge interface between the fully coupled model and the simplified one-way coupled model. (a) The slip is simulated by providing a constant velocity to the block (as shown in blue); The left side and the right side of the system are given servo-controlled stress boundary The top and bottom boundaries of the gouge are given zero displacement condition; (b) Grain displacement (z component) at t = 4ms simulated by the simplified model with one-way coupling; (c) Grain displacement (z component) at t = 4ms simulated by the fully coupled model. (d) Pore pressure change (normalized by the horizontal stress) due to slip simulated by the fully coupled model; two cross sections (y = 0 and z = 0) are shown.

stress and causing earlier slip failure driven by mechan-643 626 ical loading. They show that, for the case of a pressure₆₄₄ 627 discontinuity across the fault, the onset of slip occurs ear_{-645} 628 lier for the side with higher pore pressure, and that this646 629 onset appears to be controlled by the maximum pressure₆₄₇ 630 of both sides of the fault. Therefore, our results indicate648 631 that the fault pressure should be taken as the maximum⁶⁴⁹ 632 pressure within the fault zone in a macroscopic hydrome-633 chanical coupling analysis where the effective stress on 634 the fault is evaluated. 650 635 Natural fault zones are usually more complex than the 636

simple system considered here. In a mature fault zone,₆₅₁
multiple strands of fault gouge cores can develop (see [58]₆₅₂
and references therein), indicating there may be multi-₆₅₃
ple surfaces along which slip failure can occur. Multiple₆₅₄
gouge cores also present a significant barrier for fluid flow₆₅₅
across the fault zone. Our modeling results suggest that₆₅₆

such a fault zone would fail first on the surface where the pore pressure is highest if the friction properties for the slip surfaces are similar. The results shed new light on the use of the effective stress principle and the Coulomb failure criterion in fault stability evaluation, and thus have important implications for seismic hazard assessment of subsurface fluid injection sites.

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