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Micromechanics of wing crack propagation for different flaw properties

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Abstract

The Discrete Element Method is used to study crack propagation in intact rock from pre-existing flaws of different natures. Damage mechanisms occurring during open and closed cracks propagation are analyzed at the local scale using an innovative micromechanical investigation. Different micromechanisms are captured, due to the development of either tensile or deviatoric states of stress in the vicinity of the flaw, which are shown to be dependent on the flaw properties. In turn, crack propagation patterns, as strength, are greatly affected by the mechanical and geometrical characteristics of the initial flaw.

Keywords: Rock, Discrete Element Method, Mixed mode fracture

1. Introduction

Rock failure occurs after little plastic deformation under unconfined conditions. Such brittle failure involves catastrophic crack propagation that results from stress concentration around flaws of different natures. These flaws may result from rock genesis, *e.g.* joints between rock minerals, or loading history, *e.g.* cracks. Among the numerous possible configurations leading to fracture generation and growth, the focus is set here on a classical configuration where a rock sample is submitted to an unconfined compressive loading in presence of a unique flaw (see Fig. 1). This corresponds to mode I+II loading, and pioneering experiments based on this configuration were undertaken mainly on

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20 model materials (gypsum, PMMA, glass, etc...) as presented in [1, 2, 3]. These
 21 authors observed what is now classically denoted as *wing* or *primary cracks* and
 22 *secondary cracks*.

Figure 1: Compression of a pre-cracked sample.

23 Wing cracks are localized crack patterns propagating along the most com-
 24 pressive stress direction from the flaw tips. Secondary cracks are located near
 25 the flaw tips, forming after the wing cracks and extending in a more restrained
 26 and diffuse manner compared to the latters (see *e.g.* [2, 4]). Generally, a tensile
 27 nature is associated to wing cracks, whereas secondary cracks, sometimes de-
 28 noted as *shear cracks*, would arise from a shear mechanism [5, 6, 4]. However,
 29 some authors may state that these secondary cracks appear through the coales-
 30 cence of local tensile cracks oriented along a different direction than the wing
 31 cracks [7, 8].

32 Wing and secondary cracks have been observed with distinct shapes in model
 33 materials [1, 3, 9, 4], fragile polymers [10, 11, 12] or marble [8]. Their occurrence
 34 might be less remarkable in other rock types such as *e.g.* granite [12]. Nonethe-
 35 less, wing and secondary cracks are now commonly used by geomechanicians to
 36 describe crack propagation and coalescence in rocks [5, 8, 13].

37 Because of their consequence on the overall behavior of rock and other brit-
 38 tle materials, numerous models have been proposed to study crack propagation.
 39 Analytical derivations have been led, generally at the cost of elasticity hypothe-
 40 sis [14, 15, 16]. More complex mechanical behaviors can be handled more easily
 41 using continuous numerical modellings, such as in [17]. Nevertheless, propagat-
 42 ing cracks are difficult to describe with continuous numerical modellings; though
 43 this can still be done using meshless methods such as XFEM [18].

44

45 On the other hand, discrete multi-scale models describe efficiently by nature
46 both crack propagation and complex mechanical behavior. The inherent discrete
47 structure of rock involving a cohesive assembly of minerals as in granite, or
48 grains as in sandstone, is one reason to use such discrete models. Furthermore,
49 the Discrete Element Method for instance (DEM, [19]) has proven to be an
50 efficient modelling approach for crack propagation analysis in brittle materials
51 [20, 21, 22, 23, 24], including rock [25]. For this reason, many recent works
52 rely on the DEM to study damage in rock, in order to reproduce experimental
53 results such as acoustic emissions [26, 27] or constitutive behavior [28, 29].
54 Crack propagation from an open flaw has been studied with DEM, mainly in
55 2D [30, 12, 31]. In the regular lattice model of [30], wing cracks could be
56 generated, with a limited kink. The damage patterns obtained in [12, 31] were
57 less marked: this may arise from the heterogeneous strength parameters in these
58 models, which might be related to the differences obtained experimentally for
59 different materials.

60 One can note that less studies consider crack propagation from closed flaws.
61 Experimentally, it is difficult to generate closed flaws with controlled properties
62 [9], but some results suggest similar crack propagation patterns from open or
63 closed flaws [9, 6, 4]. Closed flaws were simulated in DEM in 2D [32] and in
64 3D [33], with, however, contradictory conclusions regarding the numerical re-
65 quirements for wing crack simulations. This will be discussed in section 5.2,
66 considering different approaches to model closed flaws. As it will be empha-
67 sized in the paper, modelling closed flaws with DEM may be biased due to the
68 spherical shape of the discrete particles if the formulation is not upgraded.

69

70 Aiming to study crack propagation in rock with various flaw properties, our
71 objective is twofold. First, we aim to propose an approach that is valid for either
72 open or closed planar flaws. Second, we seek to get micro-mechanical insights
73 on the damage mechanisms associated to wing and secondary cracks.

74 First, the DEM model used to simulate the rock matrix is presented in sec-

tion 2. The model relies on previous developments [29], and its limitations are discussed. The micro-mechanical tools are also introduced. Section 3 discusses how closed flaws are simulated in the DEM model. In section 4, crack propagation is studied considering the case of open flaws, comparing the numerical results with available experimental ones. Section 5 presents mechanically consistent simulations of crack propagation from closed flaws with different mechanical properties. Finally, section 6 provides micro-mechanical insights into wing and shear cracks propagation.

All simulations are performed with the open-source code Yade [34, 35], and the geomechanics sign convention is used throughout the whole paper, considering compressive stresses and strains as positive.

2. Rock matrix modeling

2.1. Model formulation

Rock matrix is simulated using a packing of bonded spherical discrete elements (also denoted particles in the present article). The core of the model, previously presented in [29], is to some extent similar to other DEM models for rock [25, 28]. A major difference relies in the consideration, here, of near neighbour interactions through a controlled interaction range. Indeed, interparticle bonds are created between each pair of particles A and B for which equation (1) is fulfilled:

$$D_{AB}^0 \leq \gamma_{\text{int}}(R_A + R_B) \quad (1)$$

In equation (1), R_A and R_B are the radii of the two particles, D_{AB}^0 the initial distance between the two centroids of A and B , and $\gamma_{\text{int}} \geq 1$ a parameter of the model. With such controlled near neighbour interactions, first proposed in [36], the average number of bonds per particle, N , can be predefined. This feature is motivated by the inadequate UCS/UTS ratios provided by classical DEM using spherical particles [25, 37], UCS (resp. UTS) being the uniaxial compressive (resp. tensile) strength. The mean contact number N being related to the UCS/UTS ratio [29], the γ_{int} -parameter provides the possibility to define precisely N and to simulate various rock types.

104 As an alternative, the use of clumps (rigid aggregates) of spheres has been
 105 proposed as a solution for 2D simulations [38], but the same method might
 106 lead to less significant improvements in 3D [39]. Other solutions would be to
 107 adapt the contact laws of the parallel bond model of [25], introducing up to 10
 108 parameters [39], or using the so-called *flat joint contact model* which has been
 109 developped up to now for the 2D case [40]. The use of a controlled interaction
 110 range with one scalar parameter γ_{int} provides an efficient approach simple to
 111 formulate.

112 The behavior of the medium is defined through normal and tangential in-
 113 teraction forces acting between interacting particles. Within DEM, interac-
 114 tion forces are classically computed from the relative displacement between
 115 particles. D_{AB} being the current value of the distance between the two cen-
 116 troïds, the normal force F_n is computed from the normal relative displacement
 117 $u_n = D_{AB}^0 - D_{AB}$ (u_n increases when spheres get closer to each other). Both
 118 repulsive (compressive), and cohesive (tensile), normal forces are considered. In
 119 tension, normal forces can develop up to a threshold F_n^{max} such that:

$$F_n = k_n u_n \text{ while } k_n u_n > -F_n^{\text{max}} ; F_n = 0 \text{ otherwise} \quad (2)$$

120 with $F_n^{\text{max}} = t A_{\text{int}} > 0$ computed from the tensile strength t (in Pa) and
 121 $A_{\text{int}} = \pi \min(R_A, R_B)^2$, a surface related to the interacting particles. The
 122 normal stiffness k_n is computed as a function of the particles radii and Y , a
 123 parameter of the model expressed in Pa:

$$k_n = \frac{2 Y R_A R_B}{R_A + R_B} \quad (3)$$

124 Equation (3) expresses the normal stiffness as the one of two spring series with
 125 stiffnesses $Y 2R_{A/B}$, that can be interpreted as the stiffnesses of two elastic
 126 particles. In the end, Y is related, though different, with the bulk modulus of
 127 the numerical sample.

128 The tangential local stiffness k_t is deduced from the second elastic parameter
 129 of the model, P (dimensionless) such as:

$$k_t = P k_n \quad (4)$$

130 The tangential force $\vec{F}_t$ is linearly incremented using k_t and the incremental
131 relative tangential displacement $\vec{\Delta u}_t$. Tangential forces can increase in norm up
132 to a cohesive-frictionnal threshold F_t^{max} computed from the local friction angle
133 φ and the cohesion parameter c (in Pa): $F_t^{max} = c A_{\text{int}} + F_n \tan(\varphi)$.

134 Interparticle bonds may fail through tension or shear when the normal force
135 or the tangential force reach respectively $-F_n^{max}$ or F_t^{max} . Then, the interaction
136 disappears in the tensile regime if $F_n < 0$, or keeps going in a compressive regime
137 if $F_n \geq 0$. For the latter case, the behavior becomes purely frictionnal: t and c
138 are set to zero. From this point, $F_n \geq 0$ ($F_n^{max} = 0$) and $F_t^{max} = F_n \tan(\varphi)$.
139 The same purely frictional behavior rules the interactions appearing during the
140 simulation when spheres come in strict geometrical contact (*i.e.* $\gamma_{\text{int}} = 1$).

141 An explicit time-domain integration scheme is used to solve the equations
142 of motion. The discrete elements are thus translated and rotated according to
143 the interaction forces and their resulting torques using Newton's second law.
144 Because of the dynamic formulation of the method, damping is used in the
145 model to dissipate kinetic energy, as described in the following section.

146 Table 1 presents the retained parameter values. The resulting UCS, UTS
147 and Young's modulus are respectively 70 GPa, 6 GPa and 55 GPa (see next
148 sections), which corresponds to a Carboniferous Limestone [41]. A detailed
149 presentation of the calibration process can be found in [33, 29]. Note however
150 that a complete quantitative description of this specific rock is out of the scope
of our qualitative analysis.

N	Y (GPa)	P	φ ($^\circ$)	c (MPa)	t (MPa)
12	50	1/3	18	45	4.5

Table 1: Considered model parameters for the intact rock.

151

152 2.2. Numerical damping

153 A local non-viscous damping [42] is used, introducing a damping force $\vec{F}^d$
154 in Newton's second law such that:

$$\vec{F}^d = -\alpha \operatorname{sign} \left(\Sigma \vec{F}^{(t)} \cdot \left(\vec{v}^{(t)} + \frac{dt}{2} \vec{a}^{(t)} \right) \right) \Sigma \vec{F}^{(t)} \quad (5)$$

155 $\vec{F}^d$ depends on the damping parameter $\alpha \in [0; 1]$, $\alpha = 0$ corresponding to an
156 undamped system. This damping method facilitates quasi-static simulations,
157 by dissipating kinetic energy in the model. Note that energy dissipation is also
158 included in the model through sliding and brittle failure processes. Few authors
159 present damping as an indirect modelling of other physical energy dissipation
160 sources [26, 25]. In this case, α should be considered as a model parameter
161 that would require experimental measurements such as seismic quality factor
162 for calibration. However, retained α values are in the end not consistent with
163 this approach (see *e.g.* [25]).

164 Here, damping is considered only as a convenient numerical treatment that
165 reduces computational costs, since it allows quasi-static conditions with higher
166 loading rates. Then, its possible influence on the results is assessed by simulating
167 uniaxial compression tests for different values of α , with the parameters of Table
168 1.

169 Uniaxial tests simulations consist in the loading of a parallelepipedic sample
170 of spherical particles between two rigid platens (see the Fig. 3). Deformation of
171 the sample is caused by the movement of one platen toward the other at a con-
172 stant speed. The platens are frictionless to favour a homogeneous deformation
173 inside the sample. Details about the simulation procedure and the influence of
174 the platen friction angle were given in [29]. Here, stresses deduced from the
175 force acting on the moving platen, and the one deduced from Love-Weber ho-
176 mogeneization formula [43, 44] are equal, confirming an acceptable level of the
177 homogeneity and quasi-staticity within the model.

178 As shown in Fig. 2, the pre-peak behavior is not affected by damping, but
179 the UCS increases (up to 30 % here) according to α . Failure occurs along with a
180 brutal increase in the number of broken bonds (Fig. 2). At the stress peak, the
181 perturbations induced by the rupture of one interaction trigger a chain reaction
182 leading to the failure of a set of bonds that will consequently bisect the sample
183 [26]. Such chain reaction is inhibited by the damping, thus delaying failure and
184 increasing the stress that may be reached (Fig. 2). Similar trends were reported
185 in [26, 45, 28]. Note that different simulations run with different loading rates

show the same trends, which means that quasi-staticity is ensured up to the peak in every case.

(a) Reference loading rate case. The number of broken bonds is relative to the initial number of bonds
(b) UCS for different loading rates around the reference $\dot{\epsilon} \approx 7.4 \times 10^{-4} s^{-1}$

Figure 2: Damping influence for uniaxial compression test simulation.

The significant UCS variations reveal an inherent problem of the model formulation, due to the introduced damping and the brittleness of the contact law; even though such model is quite classical for rock simulations [26, 25, 45, 28, 29]. As such, a constant low-level damping is used throughout this study: $\alpha = 0.2$, which is rather limited compared to other works: $\alpha = 0.7$ in [25], $\alpha = 0.4$ in [29]. Doing so, we approach the behavior of an undamped model, keeping reasonable computational costs.

2.3. Discrete element size influence

As, *e.g.* for computational cost reasons, the particles used in the simulations do not correspond in number and in size to real physical entities, the influence of particle size on the results has to be considered. Uniaxial compressive tests were performed on three different numerical samples (Table 2) using the parameters presented in Table 1.

Samples 1 and 2 contain around 21000 particles with a mean diameter $D \approx 22 \text{ cm}^*$. However, they do not involve the same packing due to the random

* Length units are given for consistency, but they do not matter and absolute dimensions

Designation	Number of elements	Mean diameter (m) [*]
Sample 1	20689	0.215
Sample 2	20689	0.215
Sample 3	124137	0.118

Table 2: Samples used for studying size dependency. For all samples, $L_x \approx 5.4$ m, $L_y \approx 2.4$ m, $L_z \approx 10.8$ m, and a uniform distribution of radii is used with $D_{max}/D_{min} \approx 1.86$. The (x, y, z) framework is depicted in Fig. 3, z being the loading direction.

203 generation process. Sample 3 contains around 124000 particles, with a mean
204 diameter $D' \approx 12$ cm. In accordance with Table 1, the mean coordination
205 number N is set to 12 in every case, which requires slight changes in parameter
206 γ_{int} among the different samples. The three samples contain enough particles
207 (> 10000) to ensure a representative behavior and to focus on the influence of
the mean diameter only.

Figure 3: Different samples loaded in uniaxial compression.

208

209 As shown in Fig. 4, the same macroscopic elastic stiffness is obtained what-
210 ever the mean diameter. This results from the introduction of the radii of the
211 particles in equation (3). Concerning the plastic behavior, both samples with
212 the same mean diameter D exhibit a similar strength with a difference of about
213 5% for the stress peak. However, greater differences appear for the third sample
214 that involves smaller particles with mean diameter $D' < D$. The stress peak

are not intended to correspond to physical entities.

Figure 4: Uniaxial compressive test for different samples ($D' \approx D/2$) with same parameters.

is here reduced by about 13% when the mean diameter decreases. This is related to the elastic-brittle interaction laws that induce an influence of the mean diameter on the fracture toughness, explained as follows.

For illustrative purposes, let us consider a monodisperse packing of bonded spheres of diameter D (Fig. 5). A crack of surface A_c exists in the packing, due to previous bond breakages (Fig. 5(a)). The rupture of another bond induces a growth of the crack surface by dA_c (Fig. 5(b)). Under pure tensile loading (no shear forces), the energy released during this bond breakage is equal to $E = 1/2 (F_n^{max})^2 / k_n$.

Figure 5: Crack propagation in a DEM model.

Within our model, the critical fracture energy [46] $\mathcal{G}_c = E/dA_c \propto E/D^2$ depends finally on the model parameters t , Y and on the sphere diameter D such that:

$$\mathcal{G}_c \propto \frac{t^2}{Y} D \quad (6)$$

Thus, for what concerns localized failure mechanisms, the discrete model suffers

from a size dependency: the critical surface energy is proportional to the mean diameter D , or, equivalently, the fracture toughness is proportional to $\sqrt{D}$. Using a different approach, the same conclusion has been drawn in [25]. If the toughness was to be set without any particle size-dependency, the interaction law should be modified, introducing another parameter, as suggested in [21]. Nevertheless, the following sections will show that the model still has advantages to study qualitatively crack propagation. Quantitative comparisons can also be led as long as the same discretization size is kept.

2.4. Micro-mechanical insight

For any material system, it is possible to define a symmetric tensor that expresses the power of internal forces, that is thus related to a stress tensor [47, 48, 49]. For a system made up of one particle p at equilibrium under interaction forces related to several contact points c , the symmetric internal moment tensor $\mathbf{M}^p$ [48, 49] can be used, expressed by:

$$\mathbf{M}^p = \sum_c \vec{x}^c \otimes \vec{f}^c \quad (7)$$

with $\vec{x}^c$ the position of the interaction points (from the center of the particle p) where the interaction forces $\vec{f}^c$ apply. A stress tensor at the particle scale, denoted as particle stress tensor, is then derived as:

$$\boldsymbol{\sigma}^p = -1/V^p \mathbf{M}^p \quad (8)$$

with V^p the volume of the particle (the minus sign is set to obey the geometrical sign convention). For illustration purpose, Table 3 gives two examples of $\boldsymbol{\sigma}^p$ values.

Considering a set S of particles, the related internal moment tensor $\mathbf{M}^S$ is the sum of the internal moment tensors of each particle included in S . If S contains enough particles so that it can be considered as a REV, a direct link appears between $\mathbf{M}^S$ and the Cauchy stress tensor [49], which may justify the definition of $\boldsymbol{\sigma}^p$. However, one particle can not constitute a REV for a DEM assembly, then $\boldsymbol{\sigma}^p$ is a local value that relates to the mechanical state of the assembly in a qualitative manner only.

$\sigma^p = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{3F}{2\pi R^2} \end{pmatrix}$	$\sigma^p = \begin{pmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{pmatrix}$

Table 3: σ^p for two given micro-mechanical loadings: opposite forces, or uniform pressure.

255 The field of major (most compressive) principal stresses σ_I^p computed during
 256 the pseudo elastic phase (pre-peak) of a uniaxial compression test is presented
 257 in Fig. 6 (details about such representations are given in Appendix A). Firstly,
 258 it can be observed that the principal directions of σ_I^p , at the particle scale,
 259 conform to the principal stress direction imposed at the macroscopic scale (Fig.
 6(a)). Secondly, the major principal particle stresses are here in a certain extent

Figure 6: Micro-mechanical state of the DEM model in the pseudo-elastic phase of an uniaxial compression test.

260
 261 uniform, as might be expected from such homogeneous test (Fig. 6(b)). Indeed,
 262 σ_I^p values differ from the mean $\langle \sigma_I^p \rangle$ by 50% maximum. Finally, the data

set shows that both other principal stresses are similar and negligible compared with σ_I^p , for all particles.

These results support the use of σ^p as a qualitative micro-mechanical insight to evaluate the stress distribution at the particle scale. The method will thus be used in section 6 to analyze crack propagation.

3. Rock discontinuities modeling

Pre-existing discontinuity surfaces are handled in a specific manner inside the rock model. A smooth-joint model (SJM, [50]) is applied to the *joint interactions* that concern particles located on both sides of any discontinuity surface. Using the SJM, the normal and tangential vectors of the interaction are rotated and defined according to the surface of interest, rather than upon the contact geometry of the spherical particles. The elastic-plastic constitutive relations presented in section 2 hold for joint interactions, with adequate expressions of normal and tangential relative displacements. Namely, for such interactions $u_n = (\vec{AB}^0 - \vec{AB}) \cdot \vec{n}$ with $\vec{n}$ the normal vector to the discontinuity surface, from center A to center B . $\vec{n}$ is thus different from $\vec{AB}/||\vec{AB}||$. The plastic behavior, defined according to a friction angle ϕ and a dilatancy angle ψ , is independent of the discretization of the model [33]. In order to get rid of the size dependency also in the elastic domain, the elastic local stiffnesses k_n and k_t are given by:

$$\begin{aligned} k_n &= K_n^j A_{\text{int}} \\ k_t &= K_t^j A_{\text{int}} \end{aligned} \tag{9}$$

with the interface parameters K_n^j and K_t^j expressed in Pa/m.

Compression and shear tests were conducted on a numerical rock joint to confirm the discretization-independence. A planar joint is defined in a parallelepipedic sample by assigning a SJM to all interactions located across the corresponding surface (Fig. 7). The particles lying on each side of the surface are clumped together, in order to form two rigid blocks on each side of the rock joint. With this method, different from the ones used in [51, 33], the local parameters of the joint can be tested directly without any influence of the matrix

parameters (the latter is considered as a rigid body). The joint normal and

Figure 7: Particles (spheres) and joint interactions (lines) of the rock joint discrete models. Model A describes the joint surface with particles of mean diameter $D \approx 0.63$. Model B involves particles with $D \approx 0.29$.

290

291 tangential stresses, denoted σ and τ , are directly deduced from the interact-
 292 ing forces occurring between the clumps. The normal and tangential relative
 293 displacements are denoted u and γ respectively.

294 The rock joint is first normally loaded through a compression along the $\vec{z}$
 295 axis (Fig. 7): $du = cst > 0; d\gamma = 0$. The compression is performed at constant
 296 speed up to $\sigma \approx 1$ MPa. A second phase of constant normal displacement (CND)
 297 shear mode ($du = 0; d\gamma = cst > 0$) is then applied along the $\vec{x}$ axis, Fig. 7. The
 298 constitutive behavior of the model is presented in Fig. 8. It corresponds to an
 299 elastic-plastic rock joint with two elastic stiffnesses ($K_n^{glob}; K_t^{glob}$) and a plastic
 300 behavior with constant yield surface $\tau = \sigma \tan(\phi)$ and flow rule $du^p/|d\gamma^p| =$
 301 $-\tan(\psi)$. The plastic behavior is obtained during shear displacement from
 302 $(\gamma, \tau) \approx (9 \text{ mm}, 0.7 \text{ MPa})$. Appendix B derives the equations of the curves that
 303 are plotted along the model's response in Fig. 8.

304 As shown in Fig. 8(a) and 8(b), the macroscopic elastic stiffnesses K_n^{glob} and
 305 K_t^{glob} can be considered to be unaffected by the mean diameter of the numerical
 306 sample. They depend on the micro-parameters K_n^j and K_t^j , and on the ratio
 307 between the sum of all interaction surfaces A_{int} and the apparent joint surface;
 308 which is directly related to the density of the packing. This dependence on the

Figure 8: Behavior of two rock joint discrete models involving two different samples. All computations are made with $K_n^j = 50$ MPa/m, $K_t^j = K_n^j/2$, $\phi = 35^\circ$, $\psi = 10^\circ$.

309 packing density induces a difference between K_n^j and K_n^{glob} such that: $K_n^{glob} \approx$
 310 155 ± 5 MPa/m while $K_n^j = 50$ MPa/m. However, equality between other micro-
 311 parameters and induced macro-properties is obtained: $K_t^{glob}/K_n^{glob} = K_t^j/K_n^j =$
 312 0.5, and the macro-plastic parameters ϕ and ψ are the same as those introduced
 313 at the interaction scale. This direct correspondance is remarkable in DEM and
 314 has to be pointed out.

315 4. Crack propagation from an open flaw

316 DEM simulations of open pre-existing cracks is straightforward: the particles
 317 are simply removed at the flaw location. Here, the three samples presented in
 318 Table 2 are subjected to uniaxial compression, including a flaw located at their
 319 center and persistent through the $\vec{y}$ direction. The flaw length, in the $(\vec{x}, \vec{z})$
 320 plane, is 20% of L_z .

321 4.1. Strength of pre-cracked samples with open flaws

322 The uniaxial compressive tests performed on samples with an open flaw show
 323 a continuous increase of the strength with the flaw orientation θ (Fig. 9(a)).
 324 Such trend is in qualitative agreement with experimental results obtained in [12]
 325 (Fig. 9(b)), and with discrete modelings performed by [12, 31]. One can note
 326 moreover that this result is not affected by the discretization of the model, *i.e.*
 327 the numerical assembly.

Figure 9: Strength of pre-cracked samples (open cracks) with different crack inclinations.

Quantitatively, different values of the $UCS(\theta = 90^\circ)/UCS(0^\circ)$ ratio may be obtained: around 2 in the present numerical study, 1.2 in [31] and 1.3 to 1.7 in [12]. This difference may be related to the geometry of the open flaw that is different in every case.

4.2. Crack propagation patterns from open flaws

For flaw inclinations less than 60° , distinct wing and secondary cracks can be observed (Fig. 10), resulting from the coalescence of local bond breakages (hereafter denoted as *microcracks*). This result is in accordance with previous experimental works [2, 4, 8, 13]. The location of the wing crack initiation depends on the inclination of the pre-existing flaw towards the direction of the major principal stress. For $\theta = 0^\circ$, the crack propagates from the middle of the flaw. For increasing θ -values, the initiation of the wing crack moves along the flaw to finally reach the flaw tip as observed experimentally [8, 4].

For higher inclinations ($\theta \geq 60^\circ$ here), damage first initiates with a localized pattern, at the flaw tips. Then, secondary cracks appear nearby and prevent localization, so that an unique diffuse pattern develops afterwards (Fig. 10).

In our DEM simulations, all microcracks correspond to local tensile bond failures. This is directly related to the interparticle bond strength properties which were calibrated to ensure the macroscopic behavior to be representative of a brittle rock (carboniferous limestone), with the local tensile strength that is significantly smaller than the local shear strength. Such a result would support the idea that the secondary cracks, or shear cracks, appear in fact through the coalescence of local tensile cracks oriented along another direction than the wing cracks [7, 8]. This point will be discussed in section 6.1.

Note that the obtained crack propagation patterns do not depend on the discrete element size (Fig. 11).

5. Crack propagation from a closed flaw

Closed flaws can be simulated in DEM by removing the cohesive feature of all interactions located along the flaw surface as proposed by [52, 25, 32]. For

Figure 10: Crack propagation patterns from open flaws: blue dots correspond to broken interparticle bonds locations. For σ values all in the range $[0.64 \text{ UCS}; 0.71 \text{ UCS}]$. Strengths for each case are indicated in parenthesis in corresponding labels.

Figure 11: Crack propagation pattern from open flaws, obtained for different model discretizations. At $\sigma = 21 \pm 1 \text{ MPa}$ (peak stresses of each case are indicated in label).

such approach, due to the spherical geometry of the particles, the influence of the discretization of the model is questionable since the simulated flaw surface present a roughness that depends on the size distribution of the particles located on each side of the discontinuity surface. To discuss this point, the use of the SJM is compared with this existing approach.

Again, uniaxial compression tests are considered, using the assemblies presented in Table 2. Because the flaw is closed, its mechanical properties have to be determined. All simulations were performed here with $K_n^j = K_t^j = 5$ GPa/m, $\psi = 0^\circ$ and different values of ϕ for the interactions making up the flaw surface. Whatever the approach considered, classic contact model or smooth joint model, all simulations were performed using the same non-cohesive local properties along the flaw interactions. Using the SJM, the contact geometry of these interactions was additionally rotated according to the flaw geometry (see section 3).

5.1. Strength of pre-cracked samples with closed flaws

Figure 12: Strength of the pre-cracked sample, considering two closed flaw models ($\phi = 18^\circ$). Strength of the intact sample was 71 MPa.

As expected, depending on the approach chosen for describing the closed flaw, the responses are different (Fig. 12). For low flaw inclinations ($\theta \leq 15^\circ$), the use of the SJM leads to higher strengths, compared to the classical contact model. With the SJM, the joint interactions are all oriented perpendicular to the flaw and are thus all parallel to the direction of the loading. With-

377 out the SJM, the orientations of the interactions along the flaw are randomly
 378 distributed, which leads to a lower resistance against the vertical loading. For
 379 intermediate inclinations, a drastic decrease of the strength, explained hereafter,
 380 is captured using the SJM. Without the SJM, there is a continuous, slight, in-
 381 crease of the strength according to θ , which is in fact similar to the open flaw
 382 case (see previous Fig. 9). In addition, the results obtained without the SJM are
 383 significantly affected by the discretization. Indeed, the strength variation with
 384 the flaw inclination shows different trends depending on the numerical sample
 385 (Fig. 13).

Figure 13: Strength of the pre-cracked sample for different orientations θ (see Fig. 1): closed flaw ($\phi = 18^\circ$) described removing cohesive interactions across the flaw, without SJM.

386 On the contrary, using the SJM, very few differences appear using different
 387 samples (Fig. 14(a)). Moreover, a mechanically consistent description of the
 388 flaw is clearly obtained. In every case, the strength reaches a minimum for
 389 an orientation related to the flaw friction angle (Fig. 14(b)). This results
 390 from the compressive loading, that imposes mainly vertical chains of contact
 391 forces between discrete elements (see *e.g* [53]). And, for $\theta > \phi$, sliding occurs
 392 for all joint interactions carrying vertical contact forces. Whereas there is no
 393 restriction for vertical contact forces along the flaw while $\theta \leq \phi$. For this reason,
 394 an approximatively constant strength is obtained in the inclination range $\theta \leq \phi$,
 395 while the strength of the sample is significantly reduced for $\theta > \phi$. This sound
 396 result can not be retrieved without the SJM, as shown in Fig. 12 and 13.

Figure 14: Strength of the pre-cracked sample using the SJM.

5.2. Crack propagation patterns from closed flaws

Simulating closed flaws using the SJM, crack propagation depends on both θ , the flaw inclination, and ϕ , the flaw friction.

The fracturing patterns obtained for $\phi = 0^\circ$ and different values of θ are shown in Fig. 15. No localized wing cracks form from a horizontal closed flaw, as opposed to the open flaw case. For other inclinations the patterns obtained with the closed flaw are in a certain extent similar to the ones obtained for an open flaw. Again, fracturing localizes through wing cracks for intermediate orientations ($0^\circ < \theta < 60^\circ$). However, the wing cracks here always initiate from the tips of the flaw and show a limited kink. Using another numerical method (the displacement discontinuity method), Shen *et al.* [9] showed an influence of the stiffness of the flaw surface on the curvature of the wing crack: softer flaws were shown to induce more curved wing cracks patterns, the extreme case being the case of an open flaw.

Delayed with respect to the straight localized wing cracks, zones of secondary cracks can also be observed.

For higher inclinations ($\theta > 60^\circ$ here), fracturing is diffuse throughout the whole sample, almost as if there was no flaw.

Using other values for the flaw friction angles ($\phi > 0^\circ$) demonstrates that the SJM describes wing cracks propagation for intermediate orientations if and

Figure 15: Closed crack propagation patterns at different inclinations for $\phi = 0^\circ$, using the SJM. σ values are all in the range $[0.6 \text{ UCS}; 0.7 \text{ UCS}]$. Strengths for each case are indicated in parenthesis with the corresponding labels. The closed flaw appears in black at the middle of the sample.

only if sliding occurs along the flaw ($\phi < \theta < 60^\circ$). When sliding along the flaw is prevented because $\phi \geq \theta$, diffuse damage takes place throughout the whole sample and no localized crack develops, as for high inclinations and $\phi = 0^\circ$ (Fig. 15). Such behavior is in agreement with several experiments [9, 6, 4].

When sliding is enabled ($\phi < \theta$), the fracturing pattern is modified by the frictional strength along the flaw. While increasing ϕ value, microcracks tend to propagate from the flaw tips in a unique diffuse manner. The two fracturing steps (localized wing cracks followed by diffuse secondary cracks) observed for open flaws or frictionless closed flaws can hardly be distinguished. Fig. 16 illustrates the differences observed for $\theta = 45^\circ$ with $\phi = 0$ and 30° .

Figure 16: Flaw friction angle influence on the propagation of a closed flaw ($\theta = 45^\circ$). UCS is 41 MPa for $\phi = 0^\circ$ and 46 MPa for $\phi = 30^\circ$.

This influence of the flaw friction angle emphasizes the advantage of using the SJM for simulations of closed crack propagation using spherical discrete elements. Without the SJM, the flaw friction angle can not be precisely assigned to the model, and inadequate fracturing patterns might be obtained.

This may explain why here, as in [33], wing cracks are obtained without taking into account a transfer moment law in the DEM; contrary to what has been deduced from a previous discrete study [32] where closed flaws are simulated without the SJM, by only debonding the elements. Without any friction

438 defined at the contact scale along the flaw, the strength data from this previous
 439 study suggest finally a resultant flaw friction angle belonging to $[30; 45^\circ]$ (Fig.
 440 17). According to our results, such value of the flaw friction angle prevents wing
 crack to develop.

Figure 17: Strengths of pre-cracked samples with closed flaws simulated without the SJM. From data by [32].

441

442 6. Micromechanical discussion

443 The micro-mechanical quantities presented in section 2.4 are used here to
 444 give some insights into crack propagation processes. While the model includes
 445 damage through microcracking occurring at contacts, *i.e.* at an interparticle
 446 scale, σ^P is defined at the particle scale, describing the mechanical state of one
 447 given particle surrounded by a set of contacts. However, these micro-mechanical
 448 fields represent a valuable meso-scale characterization of the stress state in the
 449 medium.

450 6.1. Micro-mechanics of open flaw propagation

451 First of all, using the micro-mechanical values, the DEM model is able to
 452 capture the stress concentration caused by the flaw, similarly to any continuous
 453 method (*e.g.* [54]). Let's consider, for instance, the sample with an open flaw
 454 inclined at 30° (Fig. 18). The heterogeneity of the major particle stress, quanti-
 455 fied by $|\sigma_I^P - \langle \sigma_I^P \rangle| / \langle \sigma_I^P \rangle$, reaches 3 here (Fig. 18(b)), while it was limited
 456 to 0.5 for a homogeneous sample (Fig. 6(b)). The presence of the pre-existing

457 flaw severely disturbs the stress distribution inside the material, with high stress
 458 concentrations at its tips and reduced stresses in some shielded areas. As shown
 459 in Fig. 10, fracturing initiates in the zones corresponding to these extreme stress
 values, with shear and wing cracks being different in nature.

(a) Major principal stress (most compressive) map (b) Variations of the major principal stress (c) Directions of the major principal stress around the flaw

Figure 18: Micro-mechanical stress for a sample with an open flaw ($\theta = 30^\circ$) under compression ($\sigma \approx 22$ MPa). See Fig. 10 for corresponding crack pattern.

460

461 On one hand, shear – or secondary – cracks tend to develop in highly com-
 462 pressed zones, *i.e.* zones sustaining high deviatoric stresses for such unconfined
 463 loading. Figure 19 depicts a direct comparison between the crack pattern and
 464 the particles sustaining the greatest deviatoric stresses $\mathbf{s}^p$ throughout the model,
 465 emphasizing the shear nature of the secondary cracks. On the other hand, wing
 466 cracks are clearly not related to shear local stresses.

467 As a matter of fact, wing cracks develop where particles sustain a tensile
 468 loading. To emphasize this point, we now consider the quantity $(\sigma_{III}^p + \sigma_I^p)$
 469 for each particle. Negative values correspond to particles with the most tensile
 470 stress σ_{III}^p negative (*i.e.* corresponding actually to tension) and greater in
 471 absolute value than the most compressive stress σ_I^p . As seen in Fig. 20, there
 472 is a very good agreement between the wing crack locations and the particles
 473 predominantly loaded in tension. First, before fracturing initiates, a lens of

Figure 19: Crack patterns and particles with $\|\mathbf{s}^p\| > 0.35 \max(\|\mathbf{s}^p\|)$ for a sample with an open flaw ($\theta = 30^\circ$, UCS = 31 MPa) under compression. The external platens are visible to show the extent of the sample.

474 tensily loaded particles exists around the flaw. Then this lens deforms into
 475 a wing pattern along which microcracking occurs. Some stress relaxation is
 476 captured after the cracks form: some particles at mid-length of the wing cracks
 477 do not obey $\sigma_{III}^p + \sigma_I^p < 0$ anymore and hence are no longer displayed (Fig.
 478 20(c) and 20(d)). Finally, it is important to note that secondary cracks are
 479 definitely not associated with tensile-loaded particles.

480 In case of high inclination ($\theta \geq 60^\circ$), the localized damage initiation evo-
 481 cated in Section 4.2 is also associated with tensile stresses. However, tensile
 482 loaded zones, *i.e.*, wing cracks do not propagate due to the proximity of highly
 483 deviatoric loaded zones where secondary cracks arise afterwards (Fig. 21).

484 In addition, the rotation of the local major principal stress directions due to
 485 the presence of the flaw is captured in Fig. 18(c). On one hand, wing cracks
 486 propagate conforming to the deflected local major principal stress directions
 487 confirming here their mode I opening nature. On the other hand, secondary
 488 cracks occur in areas with local major principal directions oriented almost ver-
 489 tically and seem to propagate along no defined direction.

Figure 20: Crack patterns and particles with $\sigma_{III}^p + \sigma_I^p < 0$ for a sample with an open flaw ($\theta = 30^\circ$, UCS = 31 MPa) under compression. The external plattens are visible to show the extent of the sample.

Figure 21: Crack patterns and particles with $\sigma_{III}^p + \sigma_I^p < 0$ for a sample with an open flaw ($\theta = 75^\circ$, UCS = 48 MPa). The external plattens are visible to show the extent of the sample.

490 6.2. Micro-mechanics of closed flaw propagation

491 In section 5, it has been shown that from closed flaw, crack propagation
 492 localizes in wing crack for more specific conditions than from open flaws. When
 493 wing cracks occur, a very good correlation can again be found between the
 494 wing crack locations and the particles sustaining a mainly tensile state of stress
 495 ($\sigma_{III}^p + \sigma_I^p < 0$) as illustrated in Fig. 22. For such cases, with $\theta > \phi$, because
 496 sliding occurs along the flaw, tensile stresses develop in the sample above each
 497 flaw tip. Again, during wing crack extension, tensile stresses develop at the tip
 498 of the wing cracks whereas stress relaxation occurs along the wing crack branch
 499 (Fig. 22(c)). Once the wing cracks have reached the sample ends, secondary
 500 cracks develop due to the concentration of compressive stresses (Fig. 23).

501
 502 For increasing ϕ values, wing crack propagation is inhibited because sliding
 503 along the flaw is reduced, limiting the development of tensile stresses at the tip
 504 of the flaw. Indeed, particles sustaining tensile stresses (with $\sigma_{III}^p + \sigma_I^p < 0$)
 505 are much fewer and are closer to the flaw with $\phi = 30^\circ$ than with $\phi = 0^\circ$, for
 506 $\theta = 45^\circ$ (Fig. 24). Ultimately, when $\phi > \theta$, tensile stresses no longer develop in

Figure 22: Crack patterns and particles with $\sigma_{III}^p + \sigma_I^p < 0$ for a sample with a frictionless closed flaw ($\theta = 30^\circ$, UCS = 41 MPa) under compression.

Figure 23: Micro-mechanical field of major principal stress σ_I^p for a closed flaw with $(\theta = 30^\circ; \phi = 0^\circ)$ at $\sigma \approx 22$ MPa. The corresponding crack pattern appears in Fig. 22(d)

Figure 24: Particles with $\sigma_{III}^p + \sigma_I^p < 0$ for a closed flaw inclined at $\theta = 45^\circ$ with different friction angles. Under ε_z 0.04 %; $\sigma_z \in [19;20]$ MPa: see the Fig. 16(a) for corresponding crack patterns.

507 the sample and wing cracks cannot grow. In such cases only a negligible amount
508 of particles with $\sigma_{III}^p + \sigma_I^p < 0$ is detected.

509

510 Despite the tensile local failure mode of all bond breakages in the model,
511 these micro-mechanical insights support the idea of different damage mecha-
512 nisms causing either primary (wing) or secondary (shear) cracks. This empha-
513 sizes the advantage of intermediate- (or meso-) scale mechanical measurements,
514 such as the particle stress tensors, for a better characterization of the stress
515 distribution inside the material.

516 7. Conclusion

517 Discrete element modeling of crack propagation in rock under uniaxial com-
518 pression has been discussed. The advantages of the model were presented as
519 well as its limitations. It has been shown that, due to the brittle nature of
520 the local interaction laws used, damping and discrete element size influence
521 quantitatively the simulated strength, but not the elastic properties.

522 The model enables to simulate explicitly both open and closed flaws with
523 various associated properties. A special attention has been paid to use an ad-
524 equate discrete model for simulating closed flaws. We showed that a realistic
525 elastic-plastic behavior with controlled properties can be obtained using a SJM
526 formulation with as little numerical bias as possible.

527 Strengths and crack propagation patterns were obtained for open and closed
528 flaws with different inclinations and favorably compared with existing experi-
529 mental results. The DEM model offers micro-mechanical insights into the differ-
530 ent damage mechanisms occurring in brittle materials. In particular, fracturing
531 localizes in the form of wing cracks at locations where tensile stresses develop.
532 Such wing cracks propagate according to the most compressive stress direction.
533 Diffuse zones of secondary cracks are shown to correspond to excess deviatoric
534 compressive stresses. The distribution of deviatoric compressive and tensile lo-
535 cal stresses depend on the nature of the flaw (open or closed) as well as on the
536 frictional strength of the flaw (if closed).

As such, the flaw friction angle affects crack propagation patterns, as well as the overall strength of the material. Ultimately, when friction increases, wing crack are inhibited and a more diffuse fracturing pattern is observed. That is, crack propagation in the intact material (the matrix) is affected by the flaw properties, and not only by those of the matrix.

The influence of the flaw properties on crack propagation and on the overall behavior emphasizes the need to use the SJM for DEM simulations of closed flaws, unless discrete particles correspond to physical entities. Such a model could then be applied to study crack coalescence under confined states. It also suggests further improvements of the DEM, by applying SJM to newly created cracks. This would be useful for bonds broken in shear mode, for which contacts still hold after bond breakage.

8. APPENDIX A: representations of σ^P field

Micro-mechanical fields such as the one depicted in Fig. 6(b) are illustrated using the following procedure. Because of the reduced thickness of the sample along the y direction ($L_y \approx L_x/2 \approx L_z/4$), plane stresses in the (x, z) plane are considered.

For a random selection of particles, principal directions of σ^P can readily be plotted at the location x, z of particles centers (plane projection of the 3D model).

A direct illustration of principal stress values for all $\sigma^P(x, y, z)$ being impossible, plane representation of another related field is made as follows. The (x, z) plane is discretized in a square grid with a cell length $dx = dz = 0.2$ m, which is around the mean diameter of particles. All particles whose center lies in one given cell x_i, z_i are identified. Then, Fig. 6, 18 and 23 rely on a micro-mechanical value of the stress inside each cell, denoted $\sigma^P(x_i, z_i)$, that is derived by summing all internal moment tensors of these particles:

$$\sigma^P(x_i, z_i) = \frac{\sum V^P \sigma^P}{dx dz L_y} \quad (\text{A.1})$$

565 If dx and dz are such that one unique cell would include the whole model,
 566 equation (A.1) corresponds to the Love-Weber formula and the macroscopic
 567 stress, at the REV scale, is obtained.

568 9. APPENDIX B: elastic-plastic behavior of a rock joint

569 Let us consider an elastic-plastic rock joint. Equation (B.1) rules the elastic
 570 behavior:

$$\begin{pmatrix} d\tau \\ d\sigma \end{pmatrix} = \begin{pmatrix} K_t^{glob} & 0 \\ 0 & K_n^{glob} \end{pmatrix} \begin{pmatrix} d\gamma^e \\ du^e \end{pmatrix} \quad (\text{B.1})$$

571 The (perfectly) plastic behavior occurs on the yield surface $\tau = \sigma \tan(\phi)$, and
 572 plastic deformation depends on the dilatancy angle ψ through the following flow
 573 rule: $du^p/|d\gamma^p| = -\tan(\psi)$ [55].

574 Being loaded under constant normal displacement shear mode ($du = 0$), under
 575 an initial value of normal stress $\sigma \neq 0$, the stress state reaches the plastic
 576 limit condition after some elastic deformation. If loading continues, any change
 577 in tangential relative displacement is fully plastic from this time: $d\gamma = d\gamma^p$.
 578 Thus $du^p = -|d\gamma^p| \tan(\psi) = -|d\gamma| \tan(\psi)$. The total normal relative displace-
 579 ment u being constant due to the imposed CND loading, the plastic dilatant
 580 behavior of the joint induces changes in the normal stress σ , as derived in equa-
 581 tion (B.2):

$$du = du^e + du^p = 0 \Leftrightarrow d\sigma/K_n^{glob} - |d\gamma| \tan(\psi) = 0 \Leftrightarrow d\sigma/|d\gamma| = K_n^{glob} \tan(\psi) \quad (\text{B.2})$$

582 This equation is plotted in Fig. 8(d). For the Mohr plane (σ, τ) , the Mohr-
 583 Coulomb plastic limit condition imposes $d\tau = d\sigma \tan(\phi)$, see Fig. 8(c). By
 584 combining this last equation with equation (B.2) the theoretical line for the
 585 plastic regime in (γ, τ) plane can be deduced, see Fig. 8(b).

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