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A displacement-softening contact model for discrete element modeling of quasi-brittle materials

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ABSTRACT

A displacement-softening contact model is proposed to simulate the failure behaviors of quasi-brittle materials using the discrete element method (DEM) based on spherical particles. The contact model is modified from the parallel bond option in the DEM code *PFC2D/3D*. By adjusting the softening coefficient, which defines the ratio between the unloading and loading contact stiffnesses in the normal component, the softening contact model can not only yield realistic compressive over tensile strength ratios as high as about 30, but also capture the highly nonlinear failure envelope at the low confining stress range, typical for rocks. Formulation of the contact model is first introduced. Uniaxial compression, direct tension and confined compression/extension tests are then performed in both 2D and 3D to illustrate the effects of the softening coefficient on the micro- and macro-scale failure mechanisms, the stress-strain behaviors and the compressive over tensile strength ratio. Calibration of the mechanical properties is conducted to identify the set of micro-scale parameters for two widely modeled rocks, Lac du Bonnet granite and Berea sandstone. Excellent agreement is achieved between the numerical simulations and the experiments in terms of the uniaxial strengths and the failure envelopes.

1. Introduction

A common issue in numerical modeling with the discrete element method (DEM),[1] based on spherical particles in a dense random packing, is that the largest compressive over tensile strength ratio (UCS/UTS) a particle assembly can attain is only about 3–5, if the interactions between the particles are limited to short-range, elasto-perfectly brittle and frictional.[2,3] The associated failure envelope generally fails to capture the high nonlinearity in the low confining stress range, typical for quasi-brittle materials such as rocks.[4,5] Such a deficiency may not be an issue for a DEM simulation if the macro-scale failure involved in the problem of interest is in a single mode, namely, either solely shear failure governed plastic flow or tensile fracturing.[6] However, rock failure in general could involve both plastic flow and tensile fracturing. The strength ratio, which can be viewed as a measure of material brittleness, then affects the transition from one mode of failure to the other. A high compressive over tensile strength ratio means that in the low confining stress range, the material is more likely to fail in tension, whereas a low strength ratio means that the material is more likely to fail in shear. In order to quantitatively model complex rock behaviors, it is therefore critical that the strength ratio as well as the failure envelope of a DEM model are properly calibrated.

Numerical strategies such as clumping/clustering particles,[7] increasing the particle interaction range[8] or using multiscale representation of the grain structure and rock fabric,[9,10] have been suggested in the literature to address the issue of the low strength ratio. Nevertheless, DEM modeling with spherical particles having only short range interactions has its appeal in its computational efficiency.

In this work, we show that a high strength ratio and the associated nonlinear failure envelope at low confinement can in fact be achieved by implementing a displacement-softening contact law within the conventional framework of soft particle DEM.[1] The discrete element code PFC2D/3D[11] is employed to illustrate the effect of the softening contact model on the macro-scale strength behaviors. The default parallel bond contact model in PFC2D/3D is modified to incorporate a softening force-displacement relationship in the normal component of the parallel bond. Only one additional parameter, the softening coefficient β, is introduced in this displacement-softening contact model.

Formulation of the displacement-softening contact model is first introduced. Effects of the softening coefficient on the uniaxial compressive and tensile strengths and the corresponding failure mechanisms in the unconfined tests are then examined. For the case where the softening coefficient yields a strength ratio of UCS/UTS ~ 10, confined extension and compression tests are performed in both 2D and 3D to

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obtain the failure envelopes. The results are compared with the Hoek-Brown and Mohr-Coulomb criteria. Finally, calibrations of the DEM model against properties similar to those of two widely studied rocks, Lac du Bonnet granite and Berea sandstone, are presented.

2. A displacement-softening contact model

A parallel bond in PFC2D/3D can be envisioned as a series of elastic springs distributed over the contact area between a pair of particles in contact. In addition to the normal and shear contact forces, bending moments can be transmitted through the contact between particles. The default parallel bond contact model includes two types of contacts acting in parallel.[3,11] They can be described by two groups of micro-scale parameters: (1) particle-particle contact (point contact): normal and shear stiffnesses, K_n and K_s ([F/L]), and the friction coefficient μ; (2) the parallel bond (area contact): apparent normal and shear stiffnesses, $\bar{k}_n$ and $\bar{k}_s$ ([F/L^3]), the normal and shear bond strengths, $\bar{\sigma}_c$ and $\bar{\tau}_c$ ([F/L^2]), and the parallel bond radius multiplier $\bar{\lambda}$. The radius multiplier $\bar{\lambda}$ defines the contact area radius for the parallel bond via $\bar{R} = \bar{\lambda}\,\min(R_A, R_B)$, where R_A and R_B are the radii of the two particles in contact. Since the stiffnesses for the two types of contact differ in dimensions, it is more convenient to specify apparent moduli as the input parameters instead. For example, the normal stiffnesses K_n for the point contact between particles and $\bar{k}_n$ for the parallel bond can be determined from,

$$K_n = \frac{4R_A R_B E_c}{R_A + R_B} \quad \bar{k}_n = \frac{\bar{E}_c}{R_A + R_B} \tag{1}$$

where E_c and $\bar{E}_c$ are the apparent moduli for the particle-particle contact and the parallel bond, respectively. Assuming compression positive, the point contact model relates the forces and displacements through,

$$F_n = -K_n\delta_n \quad \Delta F_s = -K_s\Delta\delta_s \tag{2}$$

and follows Coulomb's law of friction,

$$|F_s| \le \mu F_n \quad \text{if} \quad \delta_n \le 0, \qquad F_n = F_s = 0 \quad \text{if} \quad \delta_n > 0 \tag{3}$$

where F_n and F_s denote the normal and shear contact forces in the point contact, respectively; δ_n is the overlap ($\delta_n > 0$ indicates a gap at the contact) and δ_s is the slip between the pair of particles.

For the area contact, before reaching the softening condition, the contact forces, $\bar{F}_n$ and $\bar{F}_s$, and the bending moment, $\bar{M}$, follow incremental linear relationships with the parallel bond stretch $\bar{\delta}_n$, slip $\bar{\delta}_s$ and the angle of relative particle rotation $\bar{\theta}$,

$$\Delta\bar{F}_n = -\bar{k}_n A\Delta\bar{\delta}_n \quad \Delta\bar{F}_s = -\bar{k}_s A\Delta\bar{\delta}_s \quad \Delta\bar{M} = -\bar{k}_n I\Delta\bar{\theta} \tag{4}$$

where A and I are the cross sectional area and the moment of inertia of the parallel bond, respectively. The total force at the contact is the sum of the force components at both the point and area contacts.

The softening force-displacement relationship is implemented in the normal component of the parallel bond contact (see Fig. 1). Softening occurs when the normal contact force $\bar{F}_n$ in a parallel bond reaches a limit defined by the normal bond strength, i.e.,

$$\bar{F}_n = \bar{F}_{n\,\max} = -\bar{\sigma}_c A \tag{5}$$

The force-displacement relationship during the softening stage can be expressed as,

$$\bar{F}_n = \beta\bar{k}_n\bar{\delta}_n A - (1+\beta)\bar{\sigma}_c A \quad \text{if} \quad \bar{\delta}_n \ge \bar{\delta}_1 \tag{6}$$

where $\bar{\delta}_1$ is the bond stretch at the peak force and the softening coefficient β defines the ratio between the softening and loading stiffnesses, i.e., $\beta = \bar{k}_u/\bar{k}_l$ and $\bar{k}_l = \bar{k}_n A$. The parallel bond fails if one of the criteria below is met at the contact,

$$\bar{\delta}_n + \bar{R}|\bar{\theta}| \ge \bar{\delta}_c \tag{7}$$

$$\frac{|\bar{F}_s|}{A} \ge \bar{\tau}_c \tag{8}$$

where $\bar{\delta}_c$ is a critical bond stretch and $\bar{\tau}_c$ is the shear bond strength. Both the normal and shear forces, $\bar{F}_n$ and $\bar{F}_s$, in the parallel bond reduce to zero, when the bond fails according to Eqs. (7) or (8). The elasto-perfectly brittle case, when $\beta \to \infty$, is the default parallel bond option in PFC2D/3D and has been widely used in DEM studies in the literature.[3] The softening law described above essentially accounts for the progressive failure of the bonds and also increases the range of interaction between particles.

Breakage of a parallel bond is termed a micro-crack event here. Note that the micro-scale failure mechanisms of whether a bond fails in tension (Eq. (7)) or in shear (Eq. (8)) does not directly translate to a tensile or shear failure mechanism at the macro-scale.[12,6] In a DEM simulation, localization and coalescence of the micro-cracks to form a planar feature can be interpreted as development of a macro-crack or a shear band, while accumulation of the micro-cracks to form a cluster can be considered equivalent to growth of a crushed or damaged zone. Depending primarily on the micro-scale bond strength ratio, $\bar{\tau}_c/\bar{\sigma}_c$, the macro-scale failure mechanisms, whether it is a tensile crack, a shear band, or a damaged zone, could be a result of localization of tensile micro-cracks only, shear only or a mixture of both.[13,14] In this study, we assume that the micro-scale failure mechanism is of tensile origin, which is reasonable for quasi-brittle materials such as rocks. Therefore, we set the shear bond strength $\bar{\tau}_c$ to be much larger than the normal bond strength $\bar{\sigma}_c$ ($\bar{\tau}_c \gg \bar{\sigma}_c$). This basically renders Eq. (8) practically inapplicable here.

If we use the beam theory as an analogy for the parallel bond, $\bar{\delta}_n$ is equivalent to the elongation on the neutral plane. The normal bond failure criterion means that the bond fails if the stretch at the edge of the bond reaches the threshold value $\bar{\delta}_c$. In this model, we set $\bar{\delta}_c = \bar{\delta}_2$, i.e.,

$$\bar{\delta}_c = \bar{\delta}_2 = \frac{\bar{\sigma}_c}{\bar{k}_n}\left(\frac{1+\beta}{\beta}\right) \tag{9}$$

When the parallel bond breaks, the bond stretch $\bar{\delta}_n$ at the contact is,

$$\bar{\delta}_n = \bar{\delta}_* = \frac{\bar{\sigma}_c}{\bar{k}_n}\left(\frac{1+\beta}{\beta}\right) - \bar{R}|\bar{\theta}| \tag{10}$$

Note that $\bar{\delta}_* \le \bar{\delta}_2$ since rotational contribution is included in the normal bond failure condition (Eq. (7) or (10)). For large β, it is possible that the bond failure condition is met before the softening condition (Eq. (5)) is reached. It should be noted that in this contact model, only the coefficient β, in addition to the normal bond strength $\bar{\sigma}_c$ and $\bar{k}_n$ (or $\bar{E}_c$), is needed to describe the softening behavior.

3. Effect of the softening coefficient

3.1. Unconfined tests

A rectangular sample of $W \times H = 60 \times 120$ mm in 2D and a cylindrical sample of $D \times H = 40 \times 80$ mm in 3D are employed to investigate the effect of the softening coefficient β on the unconfined material strengths with $\beta = 0.015$, 0.1 and ∞. Particles of a uniform size distribution are generated randomly within the simulation domain. The following micro-scale parameters for the particles and contacts are chosen as the baseline: particle radii $\bar{R} = 0.8 - 1.66$ mm, density $\rho = 2630$ kg/m^3; point contact modulus $E_c = 50$ GPa, stiffness ratio $\kappa = k_n/k_s = 4.0$, friction coefficient $\mu = 0.5$; parallel bond modulus $\bar{E}_c = 50$ GPa, bond stiffness ratio $\bar{\kappa} = \bar{k}_n/\bar{k}_s = 4.0$, and contact radius multiplier $\bar{\lambda} = 1$.

The mean normal bond strength $\bar{\sigma}_c$ for each β is chosen such that the area of ΔoAB in Fig. 1 remains the same. The area of ΔoAB can be considered a nominal measure of the energy loss due to each bond breakage. Denote $\bar{U}_b$ as the nominal energy loss density,