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Calibration of DEM simulation: Unconfined Compressive Test and Brazilian Tensile Test

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Abstract. We simulate rock fracture using ESyS_Particle, which is a 3-D Discrete Element Model developed for modeling geological materials. Two types of simulations are carried out: Unconfined Compressive Test (UCT) and Brazilian Tensile Test (BTT). The results are compared to laboratory tests. Model parameters are determined on the basis of theoretical studies on the elastic properties of regular lattices and dimensionless analysis. The fracture patterns and realistic macroscopic strength are well reproduced. Also the ratio of the macroscopic strength of compression to the tensile strength is obtained numerically.

Keywords: Discrete Element Model, rock fracture, UCT, BTT.
PACS: 45.70

INTRODUCTION

Discrete Element Method (DEM) has great advantages in modeling fracture process due to its discrete nature and the possibility to reproduce dynamic processes. However, two major difficulties hinder its applications in rock mechanics. The first one is the fact that it is very time-consuming because of its step-by-step updating style and small time step is required. The second problem is parameter calibration. In the most current DEM simulations, parameters are chosen based on the trial-and-error methods. In the previous analytical studies [1], we show how to choose the spring parameters according to the given macroscopic elastic constants. However, some parameters, such as strength of the bonds, can only be investigated numerically. In this study we simulate rock fracture using ESyS_Particle, the 3-D parallel DEM software. We run two types of simulations: Unconfined Compressive Test (UCT) and Brazilian Tensile Test (BTT), and compare the results to the laboratory tests and discuss the limitations of the DEM model.

ESYS_PARTICLE MODEL

ESyS_Particle is a 3D DEM software to simulate rock mechanics, developed in the University of Queensland [2, 3, 4]. Within Esys_Particle, the recently developed Finite Deformation Method includes explicit particle rotation and a complete set of interactions between particles [3, 4]. Figure 1 shows the six interactions (normal, shearing forces, bending and twisting moment) transmitted between 3-D bonded particles. The force-displacement law between two bonded particles can be written as

$$\boldsymbol{f}_r = K_r \Delta \boldsymbol{r}, \boldsymbol{f}_{s1} = K_{s1} \Delta \boldsymbol{s}_1, \boldsymbol{f}_{s2} = K_{s2} \Delta \boldsymbol{s}_2,$$
$$\boldsymbol{\tau}_t = K_t \Delta \boldsymbol{\alpha}_t, \boldsymbol{\tau}_{b1} = K_{b1} \Delta \boldsymbol{\alpha}_{b1}, \boldsymbol{\tau}_{b2} = K_{b2} \Delta \boldsymbol{\alpha}_{b2}. \quad (1)$$

Where $\Delta \boldsymbol{r}$, $\Delta \boldsymbol{s}_i$ are the relative displacements in normal and tangent directions. $\Delta \boldsymbol{\alpha}_t$ and $\Delta \boldsymbol{\alpha}_{bi}$ are the relative angular displacements caused by twisting and bending. $\boldsymbol{f}_r, \boldsymbol{f}_{s1}, \boldsymbol{f}_{s2}, \boldsymbol{\tau}_t, \boldsymbol{\tau}_{b1}$ and $\boldsymbol{\tau}_{b2}$ are forces and torques, $K_r, K_{s1}, K_{s2}, K_t, K_{b1}$ and K_{b2} are relevant stiffness. In this study, we assume that $K_s = K_{s1} = K_{s2}$ and $K_b = K_{b1} = K_{b2}$. Detailed description of the model can be found in [3, 4, 5].

The following empirical criterion is used to judge whether or not a bond is going to break:

$$\frac{f_r}{F_{r0}} + \frac{|f_s|}{F_{s0}} + \frac{|\tau_t|}{\Gamma_{t0}} + \frac{|\tau_b|}{\Gamma_{b0}} \geq 1 \quad (2)$$

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Where F_{r0}, F_{s0}, Γ_{t0} and Γ_{b0} are thresholds for a bond to break under pure extension, pure shearing, pure bending and pure twisting respectively. We set f_r positive under extension and negative under compression such that the effects of normal force on breakage of the bond has been taken into account. Γ_{t0} and Γ_{b0} are not independent of F_{r0} and F_{s0}. In this study we choose $\Gamma_{b0} = RF_{r0}/4$ and $F_{r0} = RF_{s0}/2$ [3].

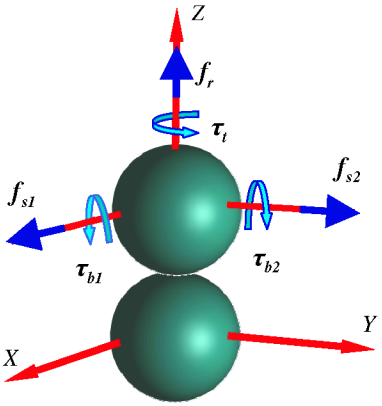

FIGURE 1. Six kinds of interactions between bonded particles. f_r is normal force, f_{s1} and f_{s2} are shear forces, τ_t is twisting torque, τ_{b1} and τ_{b2} are bending torque.

Calibration of the model parameters

As the first step to compare simulations with real experimental data, we studied analytically the relation between contact stiffness and the macroscopic elastic constants of materials [1]. For example, in 3D case of Face-Centered Cubic (FCC) packing with equal sized particles, the realistic macroscopic elastic parameters (Young's modulus and Poission's ratio) are guaranteed if the normal, shear, bending and twisting stiffnesses in DEM are chosen as:

$$K_r = \frac{\sqrt{2}ER}{2(1-2\nu)},\quad K_s = \frac{1-3\nu}{1+\nu}K_r,$$

$$K_b = \frac{\sqrt{2}ER^3}{48(1-\nu)} = \frac{(1-2\nu)R^2}{24(1-\nu)}K_r,$$

$$K_t = \frac{1-3\nu}{1+\nu}K_b = \frac{(1-2\nu)R^2}{24(1-\nu)}K_s. \qquad (3)$$

Where E, ν and R are Young's modulus and Poisson's ratio and radius of particles.

Dimensional analysis

In the DEM simulation it is desirable to choose the contact parameters in such a way that they match the material constants of the model. Sometimes these parameters are rescaled up or down, and the new group of parameters may not match the laboratory data, then other quantities should be scaled up or down accordingly. Therefore it is convenient to make dimensional analysis of the parameters. In such way we can keep the scale invariance of the model and reduce the parameters to a minimum of non-dimensionless constants [6].

The equation of Newton $F = md^2x/dt^2$, can be written in dimensionless form as $\tilde{F} = \alpha\tilde{m}d^2\tilde{x}/d\tilde{t}^2$, where $\tilde{F} = F/F_c$, $\tilde{m} = m/m_c$, $\tilde{x} = x/x_c$, $\tilde{t} = t/t_c$ and $\alpha = m_c x_c/F_c t_c^2$, x_c, m_c, t_c and F_c are the characteristic length, mass, time and force. Two models will be dynamically similar if

$$m_1 x_1/F_1 t_1^2 = m_2 x_2/F_2 t_2^2, \qquad (4)$$

where x_1, m_1, t_1, F_1 and x_2, m_2, t_2, F_2 are the characteristic length, mass, time, force of model 1 and 2 respectively. For a pure mechanical system, there are three independent dimensions: mass, length and time. Therefore if any of the three ratios between two models in Equation 4 are determined, the ratios of other quantities (such as gravitational acceleration, spring stiffness and artificial damping parameters etc) must be fixed according to Equation 4.

NUMERICAL SET UP AND RESULTS

We simulate two different laboratory tests: Unconfined Compressive Test (UCT) and Brazilian Tensile Test (BTT). In UCT test a slow uni-axial loading is applied in axial direction of a cylindrical sample and the compressive strength is measured. In BTT test, the tensile strength is measured indirectly by loading a cylindrical sample in diametrical direction.

The laboratory data (model 1) for UCT and BTT tests are listed in table 1. According to Eq. (3), the realistic spring stiffnesses are:

$$K_{r1} = \sqrt{2}E_1R_1/2(1-2\nu_1) = 1.453\times10^7\,Pa,$$
$$K_{s1} = K_{r1}(1-3\nu)/(1+\nu) = K_{r1}/3.$$

In the simulation (model 2), we may scale up or down some quantities. If we choose normal stiffness $K_{r2} = 8000Pa$, and radius of grains R_2 = 1m and density ρ_2 = 1.0 kg/m^3, we have $x_2/x_1 \approx 950-1000$, $m_2/m_1 = \rho_2 x_2^3/\rho_1 x_1^3 \approx 311475$, $t_2/t_1 \approx 2.3786\times10^4$ and $V_2/V_1 = 3.974\times10^{-2}$. Other

quantities are: D_2 = 49 m, H_2 = 139 m, V_2 = $1.6758\times10^{-7} m/s$, F_2 = 161.85 kN, which is the value we try to reproduce for UCT tests.

The initial set up of the UCT test is shown in Fig. 2 (left). It contains 44394 particles. Time step incremental is dt_2 = 0.001s, the simulation is run for N_t = 1.6 $\times10^6$ steps on a supercomputer with 64 CPUs, and it requires about 50 hours to run for each simulation.

However if the loading rate of $1.6758\times10^{-7} m/s$ is used, the calculation would be beyond the current computer power. In this simulations, we choose the rate of loading of $8\times10^{-4} m/s$, which is 5000 times larger. It is not a good strategy to increase the time step dt_2 in order to reduce computer time, since the large time step would result in fast accumulated errors.

While the spring parameters can be chosen according to the given macroscopic elastic constants (Equation 3), it is difficult to derive analytically the relation between the macroscopic strength and the strength of the bonds (F_{r0} and F_{s0}). Therefore this is investigated numerically in this study. We choose different fracture parameters F_{r0} and F_{s0}, and numerically measure the maximum load. The results are list in table 2 and 3. The data with stars mean the maximum load mostly close to the laboratory data, and the ratio between UCT strength and BTT strength is about 10, slightly larger than that of the laboratory value of 6. The fracture pattern corresponding to the star value is shown in Fig. 2b (right). The colors represent vertical displacement. The macroscopic shear fracture is clearly seen.

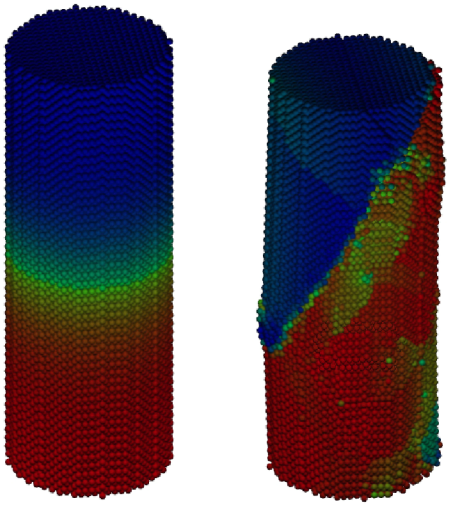

FIGURE 1. Initial set up (left) and final fracture pattern (right) for UCT tests. The color represent displacement.

It is also interesting to note from Table 2 and 3 that in UCT tests, the larger strength is observed for the large F_{s0} for the same F_{r0}, but for the same F_{s0}, the strength increases with the decrease of F_{r0}, that is, the macro-scopic strength has a positive correlation with F_{r0} and F_{s0}/F_{r0}, However, in case of BTT test, the macroscopic strength is not so sensitive to the ratio F_{s0}/F_{r0}, but has a strong dependence on F_{r0}. This difference may be explained by the fact that in UCT tests macroscopic failures are mainly caused by shear fractures and in BTT tests they are mostly controlled by tensile fractures.

SUMMARY AND DISCUSSIONS

We reproduce the fracture patterns and realistic macroscopic strength. In the laboratory tests, it is generally found that the macroscopic strength of UCT is 5-20 times larger than BTT. The UCT to BTT strength ratio of 10 is reproduced in the simulations. This ratio can be used as a good limitation to the microscopic parameters. Generally the macroscopic strength is found to have a positive correlation with F_{r0} and F_{s0}/F_{r0}. It should be bore in mind that although we reproduced the realistic strength by changing F_{r0} and F_{s0}, it is not a unique combination of parameters. A more detailed investigation on the parameters of bond breaking should be done in the future.

We conclude that using supercomputer facilities and dimensional analysis we can simulate samples with relative large number of particles and realistic materials properties. However, due to computer power, we employed a larger loading velocity in the simulations. The concern raised by such a larger loading rate is: how does the macroscopic strength change with loading velocity? To avoid this problem, one suggestion for the future simulation is that two loading rate may be used: faster loading rate during the earlier stage when the sample is relatively intact and realistic one in the latter stage when the sample is close to failure.

It became also evident that the main limitation of the computer efficiency of DEM simulations is that the currently used integration methods are unstable for larger time steps. Therefore it is a challenge for the future to develop integration methods numerically stable for large time steps, and at the same time able to reproduce the realistic dynamics of the systems.

TABLE 1. Laboratory data for UCT and BTT tests

	UCT test	BTT test
Diameter (mm)	$D_1 = 54.46$	$D_1 = 54.46$
Height (mm)	$H_1 = 147.05$	$H_1 = 147.05$
Density (kg/m^3)	$\rho_1 = 2711.6$	$\rho_1 = 2711.6$
Young Modulus (Gpa)	$E_1 = 12.33$	$E_1 = 12.33$
Poisson Ratio	$\nu_1 = 0.2\text{-}0.25$	$\nu_1 = 0.2\text{-}0.25$
Sizes of grains (mm)	$R_1 = 1$	$R_1 = 1$
Rate of loading (m/s)	$V_1 = 4.2167 \times 10^{-6}$	$V_1 = 4.2167 \times 10^{-6}$
Maximum load (kN)	$F_1 = 311$	$F_1 = 51.9$

TABLE 2. Modeled maximum load for UCT tests. Data with asterisk is the closest value to the experimental data.

F (N)	F_{s0} (N)	Maximum load (kN)
4.8	14.4	60696
4.8	24	140000
8	14.4	45758
8	20	75475
8	32	113798
14.4	4.8	18000
14.4	6.4	21432
14.4	9.6	29040
16	24	55195
64	64	164422 *
64	128	236588

TABLE 3. Modeled maximum load for BTT tests. Data with asterisk is the closest value to the experimental data

F_{r0} (N)	F_{s0} (N)	Maximum load (N)
4.8	24	6337
6.4	14.4	5000
32	64	14025
32	96	14101
64	64	17814 *
64	96	22337
64	128	27161

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