Effect of parameter evaluation on failure mode in discrete element models of rock materials

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Abstract

Numerical studies of effect of parameter evaluation on a failure mode in discrete element models of rock materials have been performed. The discrete element formulation employs spherical particles with the cohesive interaction model combining linear elastic behaviour with brittle failure. Numerical studies consisted in simulation of the uniaxial compression test using a cylindrical specimen with particle size distributions characterized by high degree of heterogeneity. Two different approaches to evaluation of micromechanical constitutive parameters have been compared. In the first approach, the contact stiffness and strength parameters depend on the local particle size, while in the second approach, global uniform contact parameters are assumed for all the contacting pairs in function of average geometric measures characterizing the particle assembly. Significant differences in the failure pattern have been observed. The uniform constitutive parameters result in localized brittle-like fractures, while a distributed damage typical for a ductile failure is obtained for the model . with local size-dependent parameters.

Keywords: discrete element method, rock, modelling, failure mode, brittle, compression, contact,

1. Introduction

Numerical programs employing the discrete element method (DEM) have achieved a status of a standard analysis tool in geomechanics. However, it seems that there is a lack of full understanding of many micromechanical mechanisms which are inherent in the DEM and influence macroscopic behaviour of DEM models. In the DEM, a material is represented by a an assembly of particles interacting among one another with contact forces. Interparticle interaction models can be based on different types of contact laws incorporating different physical effects such as elasticity, viscosity, damage and friction. Constitutive models for rocks must also take into account cohesive interaction between particles. Even using a simple model such as the linear elasticperfectly brittle model employed in the present work, a complex behaviour at the macroscopic scale can be obtained. Depending on the set of local parameters a more brittle or more ductile macroscopic behaviour can be obtained.

The main purpose of the present work is to study the influence of the evaluation method of local stiffness and strength parameters in the discrete element method on the macroscopic properties and macroscopic behaviour of the material model. Two approaches are compared. In the first approach, the stiffness and strength parameters of the contact model are assumed to depend on the size of contacting particles and are evaluated locally as certain functions of contacting pair radii. In the second approach, uniform microscopic properties are assumed in the whole discrete element assembly. The values of the global microscopic parameters can be evaluated taking into account some average particle size measure for the whole discrete element model. The discrete element models, which will be studied, have been implemented in the discrete element program DEMPack [1].

2. Discrete element method formulation

The DEM algorithm implemented in the discrete and finite element code DEMpack employs spherical particles. Particle interaction is modelled using the elastic-perfectly brittle model, in which initial bonding between neighbouring particles is assumed. When two particles are bonded the contact forces in both normal and tangential directions are calculated from the linear constitutive relationships:

$$F_n = K_n u_n, \quad \|\mathbf{F}_s\| = K_s \|\mathbf{u}_s\| \tag{1}$$

where K_n – interface stiffness in the normal direction, K_s – interface stiffness in the tangential direction, u_n – overlap ($u_n \leq 0$) or gap ($u_n > 0$) at the contact point, \mathbf{u}_s – relative displacement at the contact point in tangential direction.

Cohesive bonds are broken instantaneously when the interface strength is exceeded in the tangential direction by the tangential contact force or in the normal direction by the tensile contact force

$$F_n \ge \phi_n, \quad \|\mathbf{F}_s\| \ge \phi_s \tag{2}$$

where ϕ_n – interface strength in the normal direction, ϕ_s – interface strength in the tangential direction. Bond breakage allows us to simulate initiation and propagation of material fracture. After breakage, the contact is treated assuming a standard contact model with Coulomb friction. The normal contact force can be compressive only ($F_n \leq 0$) and the tangential contact force is limited by $\mu |F_n|$, μ being the Coulomb friction coefficient.

In the present work, we will consider two approaches in evaluation of the stiffness and strength parameters, K_n , K_s , ϕ_n and ϕ_s . In the first approach, these parameters are calculated locally, assuming that they depend on the contacting particle size [2]. Treating the cohesive bonding between two particles of the radii r_i and r_j as a bar of length L and uniform cross-sectional area A (Figure 1), where



Figure 1: Schematic connection of two particles.

$$L = r_i + r_j = 2\bar{r} , \quad A = (2\bar{r})^2$$
(3)

we obtain the following formula for the the stiffness modulus K_n :

$$K_n = 2E_c \bar{r} \tag{4}$$

where E_c is the Young's modulus of the bar material, and \bar{r} is the arithmetic mean of the particle radii

$$\bar{r} = \frac{r_i + r_j}{2} \tag{5}$$

In general, the parameter E_c cannot be identified with the Young's modulus of an equivalent continuum material E, but it can be treated as a certain scaling constant correlated with the Young's modulus of equivalent continuum material E and strongly dependent on the density of contact connections between particles. The shear stiffness of a bond between two particles K_s is computed assuming a certain value for the ratio of the normal and shear stiffness (K_n/K_s) .

Assuming maximum tensile and shear stresses in the bar connecting a pair of particles, σ_c and τ_c , the respective strengths of the bond, ϕ_n and ϕ_s , can be expressed in the following form:

$$\phi_n = \sigma_c A = 4\sigma_c \bar{r}^2 \quad \phi_s = \sigma_s A = 4\tau_c \bar{r}^2 \tag{6}$$

Equations (4) and (6) define the stiffness and strength parameters of the discrete element model as functions of the mean arithmetic radius of two contacting particles.

In the other approach, the parameters K_n , K_s , ϕ_n and ϕ_s are taken as uniform in the whole discrete element assembly [2]. Comparative studies of the formulations employing locally evaluated and global uniform parameters will require equivalent contact model parameters ensuring similar macroscopic properties.

Using the average of arithmetic means $\langle \bar{r} \rangle$ in Eq. (4) instead of \bar{r} , and the average of squares of arithmetic means $\langle \bar{r}^2 \rangle$ in Eq. (6) instead of \bar{r}^2 we obtain uniform normal contact stiffness and normal and shear strengths in the following form:

$$K_n = 2 E_c \langle \bar{r} \rangle \tag{7}$$

$$\phi_n = 4\sigma_c \left\langle \bar{r}^2 \right\rangle, \quad \phi_s = 4\tau_c \left\langle \bar{r}^2 \right\rangle \tag{8}$$

where

$$\langle \bar{r} \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} \bar{r}_i , \quad \langle \bar{r}^2 \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} \bar{r}_i^2$$
(9)

 N_c is the total number of contact pairs in the assembly, \bar{r}_i is the arithmetic mean of the radii in the *i*-th contact pair.

3. Numerical results

Comparative studies have been performed simulating the uniaxial compression test of a rock-type material using a cylindrical specimen discretized with 5868 particles with the radii 0.115– 1.240 mm. The model parameters have been taken such that obtained macroscopic properties could characterize high strength brittle rocks.

Under an increasing load the damage in the specimen is developing progressively by breakage of bonds due to excessive shear or tensile forces until a complete failure is reached. The results of simulations are presented in Figure 2 in the form of fractured specimens with distribution of the damage parameter D, which is defined for each particle as:

$$D = 1 - \frac{b^t}{b^0} \tag{10}$$

where b^t is the number of bonded contacts of a given particle at time t, and b^0 – its initial number of bonded contacts.

Figure 2a shows a failure pattern obtained for the model with local size dependent parameters, and Figure 2b presents a failure pattern predicted using the model with uniform global parameters. It can be seen that the two models have produced different failure modes. A typical brittle failure characterized by localized fracture has been predicted by the model with uniform constitutive parameters, while a distributed damage more typical for a ductile failure has been obtained with the model with local size dependent parameters.



Figure 2: Fractured specimens with distribution of the damage parameter: a) model with local evaluation of the parameters, b) model with the uniform global parameters

The difference in the failure patterns predicted for the two models can be explained analysing influence of heterogeneity of material properties on deformation behaviour. Local evaluation of the constitutive parameters increases heterogeneous nature of the model. Increasing heterogeneity in a material increases the number and magnitude of local stress concentrations. Crack formation, growth and coalescence in a more heterogenous material occur at lower average stress levels and develops more slowly and damage is more distributed than in case of a less heterogenous material, in which damage development is more rapid and more localized.

References

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