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Research paper

Mechanical properties and energy conversion of 3D close-packed lattice model for brittle rocks

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ABSTRACT

Numerical simulations using the 3D discrete element method can yield mechanical and dynamic behaviors similar to rocks and grains. In the model, rock is represented by bonded elements, which are arranged on a tetrahedral lattice. The conversion formulas between inter-element parameters and rock mechanical properties were derived. By using the formulas, inter-element parameters can be determined according to mechanical properties of model, including Young's modulus, Poisson's ratio, tensile strength (T_u), compressive strength (C_u) and coefficient of internal friction. The energy conversion rules of the model are proposed. Based on the methods, a Matlab code "MatDEM" was developed. Numerical models of quartzite were used to validate the formulas. The tested mechanical properties of a single unit correspond reasonably well with the values of quartzite. Tested T_u and C_u with multiple elements are lower than the values predicted by the formulas. In the simulation of rock failure processes, mechanical energy conversed between different forms and heat is generated, but the mechanical energy plus heat always remains constant. Variations of breaking heat and frictional heat provide clues of the fracturing and slipping behaviors of the T_u and C_u tests. The model may be applied to a wide range of geological structures that involve breakage at multiple scales, heat generation and dynamic processes.

1. Introduction

The discrete element method (DEM) was first introduced by Cundall and Strack (1979) to study the behavior of granular assemblies. The method was improved to a close-packed lattice solid model that has been used in the numerical simulation of the dynamical processes associated with earthquakes (Mora and Place, 1993, 1994). And a bonded discrete element model was proposed to simulate the behaviors of cohesive material (Mora and Place, 1998; Potyondy et al., 1996). The method permits large relative motion inside the model, non-linear behaviors and dynamic evolution (Hazzard et al., 2000). Therefore, it has been widely used in the simulation and interpretation of various geological phenomenon that involve breakage and discontinuities, such as earthquake faults with gouge (Guo and Morgan, 2007, 2008; Mora and Place, 1998), fault-propagation folding (Hardy and Finch, 2006), structural evolution of calderas (Hardy, 2008), faulting over active salt diapir (Yin et al., 2009), compaction bands (Dattola et al., 2014), growth fault (Chu et al., 2015), and extension fracture propagation in rocks with veins (Virgo et al., 2013).

In the DEM, rock is represented by an assemblage of a series of bonded discrete elements. Generally, the modeling method relies on troublesome calibration processes to determine the correct inter-element parameters (Boutt and McPherson, 2002; Cho et al., 2007; Kazerani and Zhao, 2010; Potyondy and Cundall, 2004; Schopfer et al., 2009). Tavarez and Plesha (2007) investigate the Young's modulus and Poisson's ratio of the 2D close-packed model. And Asahina et al. (2015) simulate the deformation of lattice model with arbitrary Poisson's ratio. The model has analytical elastic solutions (Griffiths and Mustoe, 2001; Hoover et al., 1974; Liu et al., 2013; Wang et al., 2000), which may provide a theoretical basis for calibration of inter-element parameters. The elastic properties of close-packed 3D lattice model have been investigated by Wang and Mora (2008). However, relations that specify bond strengths in terms of macroscopic strengths have not been reported (Ergenzinger et al., 2011). The relationship between micro inter-element properties and macro mechanical properties of 3D lattice model is not necessarily clear.

Failure processes of rock, such as faulting and earthquake dynamics, involve complicated friction, fracture, granular flow, wave

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propagation and energy conversion. Discrete element models have been applied to simulate faulting and earthquake phenomena (Abe and Mair, 2009; Fournier and Morgan, 2012; Latham et al., 2006; Mora and Place, 1993, 1994). Elastic potential energy is stored as tectonics stress when Earth's crust deforms. When a fault slips, the stored energy is suddenly released as seismic waves and heat (Mora and Place, 1993). The energy released may trigger other events and therefore have an effect on the damage incurred by the rock (Hazzard and Young, 2004; Hazzard et al., 2000; Michlmayr et al., 2013). The calculation of energy of the model provides an alternative way to study the causes of seismic wave attenuation, frictional heat generation, and failure zone evolution (Mora and Place, 1998; Place et al., 2002). Kinetic energy and elastic potential energy have been used to realize the process of faulting and induced seismicity (Latham et al., 2006), such as the stick-slip frictional behavior (Mora and Place, 1993). Place and Mora (1999) model the generation of frictional heat during faulting. However, the accuracy of the heat calculation is influenced by internal friction, and the calculated heat may be up to 10 times less than the theoretical value (Mora and Place, 1998; Place and Mora, 1999).

In this 3D discrete element model, rock is represented by bonded elements, which are arranged on a tetrahedral lattice packing. A tetrahedral unit with four elements was used to derive the conversion formulas between inter-element parameters and mechanical properties of the model. The energy conversion rules of the model are proposed, in order to simulate the energy conversion and heat generation during failure and dynamic processes of rocks. A Matlab code "MatDEM^{3D}" has been developed and numerical models of quartzite were used to validate the formulas and the model. The energy conversion and heat generation were simulated during the failure of the model. Note that, we do not stipulate a discrete element to represent a single rock grain in this paper, but rather, the assemblage of discrete elements represents a collection of spatially averaged grains (Boutt and McPherson, 2002).

2. The 3D close-packed model

The 3D discrete element model used in this study is based on the lattice solid model (Mora and Place, 1993, 1994). As shown in Fig. 1a, the elements used in the model are identical, which are hexagonal close packing (HCP). The elements interact through a spring force (Fig. 1b), in which the normal force (F_n) between two elements is defined as the product of normal stiffness (K_n) and normal relative displacement (X_n) (Hardy and Finch, 2006; Yin et al., 2009). The spring bond between two elements is originally intact, until X_n between the element pair exceeds the breaking displacement (X_b), whereupon the bond breaks, and the tensile force ceases to exist between them. However, the repulsive force still acts between the two elements when they return to a compressive contact.

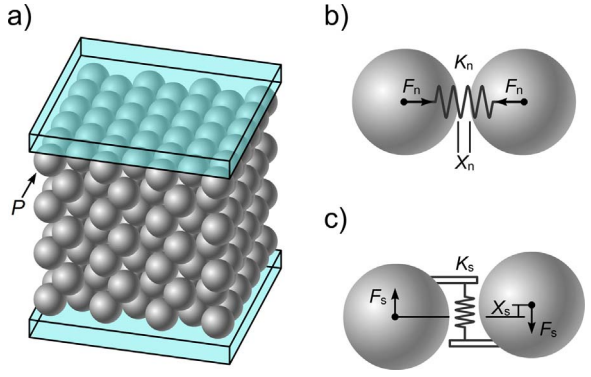

Fig. 1. (a) A 3D close-packed lattice model (hexagonal close packing). (b) Two elements are bonded by a breakable elastic spring and interact through a spring force. (c) Two elements also are bonded by a spring along the tangential direction to simulate the shear deformation and shear force.

As shown in Fig. 1c, two elements are assumed to be bonded by breakable elastic springs along the tangential direction, to simulate shear deformation and shear force. The shear relative displacement is the relative displacement of two elements along the plane perpendicular to the connection line of their centers. Similarly, the inter-element shear force (F_s) is defined as the product of shear stiffness (K_s) and shear relative displacement (X_s) (Cundall and Strack, 1979; Hardy et al., 2009). For cohesive materials, such as soil and rock, there is a cohesion between units, which is independent of the normal effective stress. Therefore, the maximum shear force (F_{Smax}) of an intact bond allowed by Coulomb friction is:

$$F_{S\,\max} = Fs_0 - \mu_p \cdot F_n \tag{1}$$

where Fs_0 is the inter-element initial shear resistance; μ_p is the inter-element coefficient of friction; F_n is the normal force (compressive force is negative). The Fs_0 is the maximum shear force, when the normal force (F_n) is zero. The shear relative displacement and shear force increase with increasing external shear force. The intact bond between two elements will break when the external force exceeds the F_{Smax} of Eq. (1). Then, the magnitude of the shear force (F_S) is limited to be less than or equal to the maximum shear force (F_{Smax}') of the broken bond, $-\mu_p \cdot F_n$. When the bond is broken and the magnitude of external shear force exceeds the limit F_{Smax}', two elements begin slipping, and the slipping friction between the element pair is F_{Smax}'.

3. Mechanical properties of the 3D model

3.1. Deformation of basic tetrahedral unit

The basic tetrahedral unit shown in Fig. 2a is used to investigate the mechanical properties of the model. In the unit, four identical elements are bonded to each other. The centers of the elements 1–4 are originally located at points A~D, respectively. In Fig. 2b, the z-coordinate of elements 2, 3 and 4 is fixed to simulate rigid smooth boundary. An external force, Fz acts on the element 1, which moves upward by a very small displacement dz to point A'. In response to the tensile force, the centers of the elements 2, 3 and 4 move toward the center point (O) of the equilateral triangle BCD to points B', C' and D', respectively. When the displacements are very small, the deformation of the tetrahedral unit has analytical solutions, and dz, X_{n1}, X_{s1} and X_{n2} can be expressed as (details in Appendix A):

$$dz = \frac{5K_n + K_s}{9K_n(K_n + K_s)} \cdot Fz \tag{2a}$$

$$X_{n1} = \frac{\sqrt{6}(3K_n + K_s)}{18K_n(K_n + K_s)} \cdot Fz \tag{2b}$$

$$X_{s1} = \frac{2\sqrt{3}K_n}{9K_n(K_n + K_s)} \cdot Fz \tag{2c}$$

$$X_{n2} = -\frac{\sqrt{6}(K_n - K_s)}{18K_n(K_n + K_s)} \cdot Fz \tag{2d}$$

3.2. Young's modulus and Poisson's ratio

By using Eqs. (2d) and (2a), the normal strains of the unit along the x-direction (ε_{xx}) and z-direction (ε_{zz}) are defined by:

$$\varepsilon_{xx} = \frac{X_{BO}}{l_{BO}} = \frac{X_{n2}}{l_{BC}} = -\frac{\sqrt{6}(K_n - K_s)}{18K_n(K_n + K_s)} \cdot \frac{Fz}{d} \tag{3a}$$

$$\varepsilon_{zz} = \frac{dz}{l_{AO}} = \frac{\sqrt{6}(5K_n + K_s)}{18K_n(K_n + K_s)} \cdot \frac{Fz}{d} \tag{3b}$$

where d is the edge length for the tetrahedral lattice unit, i.e. the diameter of element; X_{BO} is the displacement of element 2 along line