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A fast adhesive discrete element method for random packings of fine particles

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HIGHLIGHTS

- To accelerate DEM, scaling laws are proposed to reduce particle Young's modulus and the surface energy.
- An inversion method is presented to quickly set the parameters in fast adhesive DEM.
- The fast DEM retains both micro- and macroscopic properties of adhesive packings.

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ABSTRACT

Introducing a reduced particle stiffness in discrete element method (DEM) allows for bigger time steps and therefore fewer total iterations in a simulation. Although this approach works well for dry non-adhesive particles, it has been shown that for fine particles with adhesion, system behaviors are drastically sensitive to the particle stiffness. Besides, a simple and applicable principle to set the parameters in adhesive DEM is also lacking. To solve these two problems, we first propose a fast DEM based on scaling laws to reduce particle Young's modulus, surface energy and to modify rolling and sliding resistances simultaneously in the framework of Johnson-Kendall-Roberts (JKR)-based contact theory. A novel inversion method is then presented to help users to quickly determine the damping coefficient, particle stiffness and surface energy to reproduce a prescribed experimental result. After validating this inversion method, we apply the fast adhesive DEM to packing problems of microparticles. Measures of packing fraction, averaged coordination number and distributions of local packing fraction and contact number of each particle are in good agreement with results simulated using original value of particle properties. The new method should be helpful to accelerate DEM simulations for systems associated with aggregates or agglomerates.

1. Introduction

In multiphase and granular flows, discrete element method (DEM) has been widely used to model particle-particle interaction and accurately predict the motion of individual particles (Cundall and Strack, 1979; Tsuji et al., 1993; Zhu et al., 2008; Marshall and Li, 2014; Sundaresan et al., 2018; Xiao et al., 2016). For soft-sphere DEM, Young's modulus of particles used in the simulation is usually much smaller than its real value. Therefore, it is reasonable to select a much larger time step to resolve inter-particle collisions, which considerably reduces the computation cost (Tsuji et al., 1993). For systems with non-adhesive particles, the stiffness can be reduced by several orders without altering the simulation results. For instance, in fluidization systems, the flow patterns, both the shape and size distributions of bubbles, are reported to be insensitive to the particle stiffness (Moreno-Atanasio et al., 2007; Gu et al., 2016). For a collision between two particles, the post-collisional velocity is also mainly determined by the damping coefficient rather than the particle stiffness (Marshall, 2009).

However, for fine particles with van der Waals adhesion or wet particles with cohesion, a reduction of stiffness in DEM models can substantially change the simulation results (Gu et al., 2016). Intuitively, with a smaller stiffness, the particles in contact tend to have a larger deformation along the direction of compression and an enlarged area of the contact region, which leads to an overestimation of the adhesive effect (Kobayashi et al., 2013; Liu et al., 2016a). To counterbalance the deviation that arises from the reduced stiffness, a modification of the adhesive force is often needed. Kobayashi et al. (2013) simply regarded the adhesive force as a

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constant external force and then reduced it to recover the original value of the critical sticking velocity. Similar ideas were adopted by Gu et al. (2016) and by Hærvig et al. (2017), who modified the van der Waals force between particles to conserve the cohesive energy during a quasi-static two-particle collision, and by Washino et al. (2018) who derived a series of generic scaling to modify external attractive forces. In these previous studies, the adhesive force model has been modified based on the simple case of binary collision, thus is suitable only for the collision-dominated process, like fluidization process with a velocity much higher than the minimum fluidization value (Kobayashi et al., 2013; Gu et al., 2016) or powder flow in a mixer with high rotating rate (Washino et al., 2018).

An important but missing component in current adhesive DEM with reduced stiffness is its applicability to the problem associated with particle aggregates. These systems are actually quite ubiquitous in both industry and nature, such as coagulation of particles in interstellar space and protoplanetary disks (Chokshi et al., 1993; Dominik, 1997), formation of dust cake during capture of aerosol particles (Li and Marshall, 2007; Chen et al., 2016b; Wei et al., 2018), packing of adhesive particles around or below the minimum fluidization velocity (Valverde et al., 2004; Hakim et al., 2005; Liu et al., 2015; Luo et al., 2017), etc. In these situations, it is of central importance to correctly predict both dynamic evolution and static structures of aggregates. For instance, it has been reported that coagulation between aggregates and particles dominates the growth from submicron-sized grains to kilometer-size planetesimals (Dominik, 1997), and the structures of dendrites (chainlike agglomerates) on fiber surfaces have a remarkable influence on capture efficiency of aerosol particle (Li and Marshall, 2007; Payatakes and Gradoń, 1980). Previous work has shown that packing of adhesive particles can be mechanically stable with packing fraction as low as 0.15 and coordination number close to 2 (Liu et al., 2015, 2016b, 2017b). Generally, a loose aggregate can be stable due to: (1) attractive forces that prevent the detaching of two contact particles (known as necking effect); (2) a rolling resistance and a sliding friction, arising from the asymmetrical distribution of the stress and surface roughness in the contact area, respectively. These resistances prevent the particle from rolling or sliding over its neighboring particles and should be properly calculated when reduced stiffness is used.

In this paper, we demonstrate how to properly consider rolling and friction resistances in the framework of adhesive DEM based on Johnson-Kendall-Roberts (JKR) contact theory (Johnson et al., 1971) with reduced stiffness. It allows us to reproduce essentially the same packing structures as those calculated with real particle properties. Before showing a mass of packing structures in Section 4, we first briefly introduce the adhesive DEM based on JRK contact theory and rigorously derive a simple scaling law for use of reduced stiffness in Section 2. In Section 3, we propose an inversion procedure, by which the parameters in DEM can be set according to a prescribed particle-wall collision result.

2. Modeling framework

2.1. Adhesive DEM based on JKR contact theory

The discrete element method is a framework that solves Newton's second law of each particle. The particles are regarded as soft bodies and the forces and torques between contact particles are resolved. In the JKR-based models proposed in our previous work (Li and Marshall, 2007; Marshall, 2009; Li et al., 2011), the normal force F^N, the sliding friction F^S, the twisting torque M^T, and the rolling torque M^R acting on particle i from its neighboring particle j can be expressed as

$$F_{ij}^N = -4F_C\left(\hat{a}_{ij}^3 - \hat{a}_{ij}^{3/2}\right) - \eta_N \boldsymbol{v}_{ij}\cdot\boldsymbol{n}_{ij}, \tag{1a}$$

$$F_{ij}^S = -\min\left[k_T\int_{t_0}^{t}\boldsymbol{v}_{ij}(\tau)\cdot\xi_S \mathrm{d}\tau + \eta_T\boldsymbol{v}_{ij}\cdot\xi_S,\ F_{ij,crit}^S\right], \tag{1b}$$

$$M_{ij}^T = -\min\left[\frac{k_T a^2}{2}\int_{t_0}^{t}\boldsymbol{\Omega}_{ij}^T(\tau)\cdot\boldsymbol{n}_{ij}\mathrm{d}\tau + \frac{\eta_T a^2}{2}\boldsymbol{\Omega}_{ij}^T\cdot\boldsymbol{n}_{ij},\ M_{ij,crit}^T\right], \tag{1c}$$

$$M_{ij}^R = -\min\left[4F_C\hat{a}_{ij}^{3/2}\int_{t_0}^{t}\boldsymbol{v}_{ij}^L(\tau)\cdot\boldsymbol{t}_R\mathrm{d}\tau + \eta_R\boldsymbol{v}_{ij}^L\cdot\boldsymbol{t}_R,\ M_{ij,crit}^R\right]. \tag{1d}$$

The first term in the right-hand side of the normal force is derived from the JKR contact theory. It combines the effects of van der Waals attraction and elastic deformation of contact particles (Johnson et al., 1971). The scale of the first term is set by the critical pull-off force, $F_C = 3\pi R_{ij}\gamma$, where γ is the surface energy of the particle, $R_{ij} = \left(r_{p,i}^{-1} + r_{p,j}^{-1}\right)^{-1}$ is the effective particle radius, $r_{p,i}$ is the radius of particle i. $\hat{a}_{ij}$ is calculated by normalizing the radius of the contact area a_{ij} with its value at the zero-load equilibrium state $a_{ij,0}$, given as $a_{ij,0} = \left(9\pi\gamma R_{ij}^2/E_{ij}\right)^{1/3}$ (Marshall, 2009), E_{ij} is the effective elastic modulus. The second term of Eq. (1a) is the viscoelastic dissipation, which is in proportion to the rate of deformation $\boldsymbol{v}_{ij}\cdot\boldsymbol{n}_{ij}$, with $\boldsymbol{n}_{ij}$ being the unit vector pointing from the centroid of particle i to that of particle j and $\boldsymbol{v}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$ the relative particle velocity. The normal dissipation coefficient $\eta_N = \alpha\sqrt{m^* k_N}$ is described in Marshall (2009), Tsuji et al. (1992) with the coefficient α related to the coefficient of restitution e. $m^* = \left(m_i^{-1} + m_j^{-1}\right)^{-1}$ is the effective mass of the two contacting particles, where m_i is the mass of particle i. The normal elastic stiffness k_N is expressed as $k_N = \frac{4}{3}E_{ij}a_{ij}$ and the tangential stiffness k_T is given as $k_T = 8G_{ij}a_{ij}$. The effective elastic and shear moduli E_{ij} and G_{ij} are both functions of particle's Young's modulus E_i and Poisson ratio σ_i:

$$\frac{1}{E_{ij}} = \frac{1-\sigma_i^2}{E_i} + \frac{1-\sigma_j^2}{E_j},\quad \frac{1}{G_{ij}} = \frac{2-\sigma_i}{G_i} + \frac{2-\sigma_j}{G_j}, \tag{2}$$

where $G_i = E_i/2(1+\sigma_i)$ is the particle's shear modulus. The sliding friction, the twisting torque, and the rolling torque (Eqs. (1b)–(1d)) are all calculated using spring-dashpot-slider models, where $\boldsymbol{v}_{ij}\cdot\xi_S, \boldsymbol{\Omega}_{ij}^T$, and $\boldsymbol{v}_{ij}^L$ are the relative sliding, twisting, and rolling velocities, and ξ_S and $\boldsymbol{t}_R$ are the unit vectors in the directions of sliding and rolling, respectively. When these resistances reach their critical limits, $F_{ij,crit}^S, M_{ij,crit}^T$ or $M_{ij,crit}^R$, a particle will irreversibly slide, twist or roll relative to its neighboring particle. The critical limits are expressed as (Marshall, 2009):

$$F_{ij,crit}^S = \mu F_C\left|4\left(\hat{a}_{ij}^3 - \hat{a}_{ij}^{3/2}\right) + 2\right|, \tag{3a}$$

$$M_{ij,crit}^T = \frac{3\pi a_{ij}F_{ij,crit}^S}{16}, \tag{3b}$$

$$M_{ij,crit}^R = 4F_C\hat{a}_{ij}^{3/2}\theta_{crit}R_{ij}. \tag{3c}$$

Here μ is the friction coefficient and θ_{crit} is the critical rolling angle. One can set their values according to experimental measurements (Sümer and Sitti, 2008).

2.2. Accelerating adhesive DEM using reduced stiffness

The typical collision time t_C, which is defined as the time associated with the elastic response during the collision between two particles, can be generally estimated as $t_C = r_p\left(\rho_p^2/E^2U\right)^{1/5}$ (Li and Marshall, 2007). To resolve the collision, one should use a time step $\mathrm{d}t_C = f_C t_C$ with f_C much less than unity. Acceleration of the simulation can be achieved by choosing a reduced Young's