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DISCRETE AND CONTINUUM MODELLING OF GRANULAR FLOW

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Abstract This paper analyses three popular methods simulating granular flow at different time and length scales: discrete element method (DEM), averaging method and viscous, elastic-plastic continuum model. The theoretical models of these methods and their applications to hopper flows are discussed. It is shown that DEM is an effective method to study the fundamentals of granular flow at a particle or microscopic scale. By use of the continuum approach, granular flow can also be described at a continuum or macroscopic scale. Macroscopic quantities such as velocity and stress can be obtained by use of such computational method as FEM. However, this approach depends on the constitutive relationship of materials and ignores the effect of microscopic structure of granular flow. The combined approach of DEM and averaging method can overcome this problem. The approach takes into account the discrete nature of granular materials and does not require any global assumption and thus allows a better understanding of the fundamental mechanisms of granular flow. However, it is difficult to adapt this approach to process modelling because of the limited number of particles which can be handled with the present computational capacity, and the difficulty in handling non-spherical particles. Further work is needed to develop an appropriate approach to overcome these problems.

Keywords granular flow, hopper flow, discrete element method, average method, continuum approach

1. Introduction

The dynamic behavior of granular materials is very complicated. As with solids, they can withstand deformation and form heaps; as with liquids, they can flow; as with gases, they exhibit compressibility. These features give rise to another state of matter that is poorly understood (de Gennes, 1999). Corresponding to the fluid- and solid-like modes, different regimes have been identified in the past: quasi-static regime, rapid flow regime and a transitional regime that lies in between. To describe the flow behavior in these regimes, different approaches at different time and length scales have been developed in the past. Generally speaking, they can be categorize into two length scales: microscopic and macroscopic. At a microscopic or particle scale, granular material is a discrete system whose physical properties are discontinuous with respect to position and time. On the other hand, at a macroscopic or bulk scale, granular material is a continuum system whose physical properties are continuous. Based on such considerations, different approaches have been proposed to describe granular material at the two distinct scales.

An important simulation approach which can describe granular flow at a particle scale is the so-called discrete element method (DEM) originally developed by Cundall and Strack (1979). The method considers a finite number of discrete interacting particles, and every particle in the considered system is described by Newton's equations of motion related to translational and rotational motions. The motion of every particle is traced and the gradients of translation and rotation of a particle are determined in terms of the forces and the torques exerted on it. DEM-based simulation has been used to study the physics of granular materials (e.g., Herrmann & Luding, 1998; Kishino, 2001; Zhu et al., 2004), and applied to investigate various engineering problems such as mixing (Wightman et al., 1998; Stewart et al., 2001), grinding/granulation (Yamane et al., 1998; Yang et al, 2003) and hopper flow (Ristow, 1992; Langston et al., 1995a; Zhu & Yu, 2004).

By use of a proper averaging procedure, the discrete system considered above can be transferred into a corresponding continuum system. Extensive research has been carried out to develop such averaging methods. The methods thus far proposed can be divided into three classes: volume average (Drescher & de Josselin de Jong, 1972; Rothenburg & Selvadurai, 1981), time-volume average (Walton & Braun, 1986; Zhang & Campbell, 1992) and weighted time-volume average (Babic, 1997; Zhu & Yu, 2002). Based on a proper averaging method, the macroscopic quantities such as density, velocity and stress can be obtained in terms of the microscopic quantities such as velocities of particles, and interaction forces and torques between particles. The combined approach of DEM and averaging method has been applied to the macro-dynamical analysis of granular flows (e.g., Langston et al., 1995a; Potapov & Campbell, 1996; Zhu & Yu, 2005b), and has been used to study the intrinsic characteristics of granular materials such as the constitutive relationship under various flow conditions (Oda & Iwashita, 2000; Alonso-Marroquin & Herrmann, 2005).

Granular material can also be modeled by continuum approach on a macroscopic scale. In the continuum approach, the macroscopic behavior of granular flow is described by the balance equations facilitated with constitu-

tive relations and boundary conditions. In the past, two continuum models developed based on the plasticity theory and kinetic theory of molecular dynamics have extensively been used to study the dynamic behavior of granular materials (Lun et al., 1984; Campbell, 1990; Nedderman, 1992). They have been illustrated to be applicable to quasi-static and rapid flow regimes, respectively. Recently, these approaches have also been developed to study granular flows in the transitional regime. An important method is the viscous, elastic-plastic continuum model. It has been extensively applied to various cases (e.g., Wu, 1990; Oda & Iwashita, 2000).

This paper analyses the three popular methods simulating granular flows at a microscopic and macroscopic scales: discrete element method, averaging method and viscous, elastic-plastic continuum model. The mathematical models of these methods and their applications to hopper flows are considered. The advantages and disadvantages involved in the theories and applications of these methods are discussed.

2. Mathematical Models

2.1 Discrete element method

In the DEM simulation, a granular material is modeled based on a finite number of discrete, semi-rigid spherical or polygon shaped particles interacting by means of contact or non-contact forces, and the translational and rotational motions of every single particle in a considered system are described by Newton's laws of motion. For simplicity, our present study is limited to coarse spherical particle systems in which the effect of interstitial fluid and non-contact forces such as the van der Waals and electrostatic forces can be ignored. Therefore, the governing equations for translational and rotational motion of particle *i* can be given by

$$m_i \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \sum_j \mathbf{f}_{ij} + \mathbf{f}_i^{\mathrm{b}} + m_i \mathbf{g} \,, \tag{1}$$

$$I_i \frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \sum_j \mathbf{m}_{ij} + \mathbf{m}_i^{\mathrm{b}} \,. \tag{2}$$

The most complicated issue with this method is probably the calculation of the interaction forces and torques between particles. Various approaches have been proposed to model the interparticle forces. One of the most popular force models is developed based on the consideration of contact elastic force and viscous contact damping force (Langston et al., 1995a; Tanaka et al., 2002; Zhu & Yu, 2003). In general, the total interaction force between particles can be expressed as a normal component and a tangential one. The normal force includes elastic and damping components. The tangential force is described by static and dynamic frictions. Prior to the relative sliding of the contacting particles, the tangential force is described by the static force including two components corresponding to the normal elastic and damping forces respectively. When particles at contact start to slide relatively, the tangential force is described by the dynamic friction, usually, given by the Coulomb friction model. The contact between two particles is not a single point but is a finite area due to the deformation of both particles. The interparticle forces act over the contact region between particles rather than the mass centre of the particles, and they will generate a torque. The total torque includes two parts. One of the two parts, causing particle *i* to rotate, is contributed by the tangential components of the traction distribution. Another, often referred to as the rolling friction torque, is contributed by the asymmetrical normal components of the traction distribution. It provides a resistance to relative rolling motion between particles. Based on the forms of their stiffness parameters, the force models can be divided into two classes: linear model and nonlinear model. It is still open for discussion which model is better. The detailed equations about the nonlinear model for spherical particles are listed in Table 1.

Table 1 Equations for the calculation of interparticle force and torque

Force and torque	Equations
Normal elastic force $\mathbf{f}_{ij}^{ne}$	$\frac{4}{3}E_i^*\sqrt{R_{ij}^*}\left(\delta_{ij}^n\right)^{\frac{3}{2}}\mathbf{n}_{ij}$
Normal damping force $\mathbf{f}_{ij}^{nd}$	$-c_{ij}^n\left(8m_{ij}E_i^*\sqrt{R_{ij}^*\delta_{ij}^n}\right)^{\frac{1}{2}}\bar{\mathbf{v}}_{ij}^n$
Tangential elastic force $\mathbf{f}_{ij}^{te}$	$-\mu_{ij}\left\|\mathbf{f}_{ij}^{ne}\right\|\left(1-\left(1-\min\left(\left\|\mathbf{v}_{ij}^t\right\|,\ \delta_{ij}^{\max}\right)/\delta_{ij}^{\max}\right)^{\frac{3}{2}}\right)\hat{\mathbf{v}}_{ij}^t$
Tangential damping force $\mathbf{f}_{ij}^{td}$	$2c_{ij}^t\left(1.5\mu_{ij}m_{ij}\left\|\mathbf{f}_{ij}^{ne}\right\|\sqrt{1-\left\|\mathbf{v}_{ij}^t\right\|/\delta_{ij}^{\max}}/\delta_{ij}^{\max}\right)^{\frac{1}{2}}\bar{\mathbf{v}}_{ij}^t$
Coulomb friction $\mathbf{f}_{ij}^t$	$-\mu_{ij}\left\|\mathbf{f}_{ij}^{ne}\right\|\hat{\mathbf{v}}_{ij}^t$
Friction torque $\mathbf{m}_{ij}^t$	$C_{ij}\times\mathbf{f}_{ij}^t$
Rolling friction torque $\mathbf{m}_{ij}^n$	$-\min\left\{\mu_{r,ij}\left\|\mathbf{f}_{ij}^{ne}\right\|,\ \mu_{r,ij}^{'}\left\|\boldsymbol{\omega}_{ij}^n\right\|\right\}\hat{\boldsymbol{\omega}}_{ij}^n$

where $R_{ij}^* = \left(R_iR_j\right)/\left(R_i+R_j\right)$, $E_i^* = E_i/\left[2(1-\nu_i^2)\right]$, $\delta_{ij}^n = R_i+R_j-\left|\mathbf{r}_j-\mathbf{r}_i\right|$, $\bar{\mathbf{v}}_{ij}^n = (\mathbf{v}_{ij}\cdot\mathbf{n}_{ij})\cdot\mathbf{n}_{ij}$, $\bar{\mathbf{v}}_{ij}^t = (\mathbf{v}_{ij}\times\mathbf{n}_{ij})\times\mathbf{n}_{ij}$, $\mathbf{v}_{ij} = \mathbf{V}_i-\mathbf{V}_j+\boldsymbol{\omega}_i\times\mathbf{C}_{ij}-\boldsymbol{\omega}_j\times\mathbf{C}_{ji}$, $\mathbf{n}_{ij} = \left(\mathbf{r}_i-\mathbf{r}_j\right)/\left|\mathbf{r}_i-\mathbf{r}_j\right|$, $\hat{\mathbf{v}}_{ij}^t = \mathbf{v}_{ij}^t/\left|\mathbf{v}_{ij}^t\right|$, $\hat{\boldsymbol{\omega}}_{ij}^n = \boldsymbol{\omega}_{ij}^n/\left|\boldsymbol{\omega}_{ij}^n\right|$, $\delta_{ij}^{\max} = \mu_{ij}\delta_{ij}^n(2-\nu_i)/[2(1-\nu_i)]$

To track the evolution of the positions of particles, their initial positions and velocities are first given. The initial information is then used to calculate the interparticle forces and torques for each contact by means of the force and torque models listed in Table 1. Solving Eqs. (1) and (2) by use of a numerical scheme gives new positions and velocities of these particles at time Δt. The time step, Δt, should be set smaller than a certain critical value (Langston et al, 1995b). Using the new particle positions and velocities, the calculation cycle is repeated in the next time step. Therefore, the evolution of the position of each particle can be determined.

2.2 Averaging method

By use of a proper averaging procedure, the discrete system considered above can be transferred into a corre-