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Hybrid discrete-continuum model for granular flow

Xizhong Chen\textsuperscript{a,b} and Junwu Wang\textsuperscript{a}\textsuperscript{*}

\textsuperscript{a} State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, P. R. China
\textsuperscript{b}University of Chinese Academy of Sciences, Beijing, 100490, P. R. China

Abstract

We present a hybrid discrete-continuum model for multi-scale simulation of granular flow. In this method, the domain is decomposed into a discrete sub-domain, where individual particles are tracked using discrete element method, and a continuum sub-domain is solved using the Navier-Stokes equation combined with kinetic theory of granular flow. The spatial coupling between continuum method and discrete method is achieved through an overlap region, in which both methods’ variables are shared with each other. The feasibility of the hybrid discrete-continuum model is demonstrated through the simulation of a velocity-driven granular Poiseuille flow with mono-disperse, smooth (frictionless) particles.

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Nomenclature

\begin{tabular}{ll}
  \textit{dp} & particle diameter, m \\
  \textit{e} & coefficient of restitution between particle-particle interaction \\
  \textit{g_0} & radial distribution function \\
  \textit{p_s} & particle pressure, Pa \\
\end{tabular}

* Corresponding author. Tel.: +86 10 82544842; fax: +86 10 62558065.

E-mail address: jwwang@ipe.ac.cn.
Granular material is a collection of macroscopic solid particles such as sand, glass and coal. The flow of granular material is of important scientific and industrial interest owing to its common occurrence in various industries and in nature. To achieve an optimal design and successful operation of these kinds of devices, a correct assessment of the underlying principles of the granular flow fields is necessary. Unfortunately, the mechanics of granular material is not well understood at the present time due to the lack of fundamental knowledge in the granular rheological properties. The scale-up, design and optimization of these equipments are still based largely on experience and empirical rules in industries [1].

Nevertheless, researchers have developed theories and methods to represent the flow regimes observed by experiments. Two approaches that have been frequently used to model the granular flow are macroscopic continuum approach and microscopic discrete approach [2]. The former treats the granular material as continuous medium, conservation equations of mass, momentum and granular energy with kinetic theory for constitutive relations are used to track the spatial-temporal variations of granular matters[3]. Continuum method normally requires much less computational resources and therefore can be used to study the systems which contain a very large number of particles that is currently far beyond the reach of discrete models. However, the discrete character of the particles is lost in the continuum method and the accuracy of the simulation results depends on the constitutive relations. The limitation can be overcome by discrete approach such as discrete element method (DEM)[4], in which particles are tracked individually according to Newton’s laws of motion with detailed particle-particle and particle-wall collisions. Moreover, the particle scale attributes such as shape, size distribution and cohesive characteristics can easily be incorporated into the discrete method. On the other hand, the main drawback of discrete method is the high computational demands, which restricts its applications to small scale, fundamental investigations. Therefore, neither class of the two approaches is superior to the other in all respects, both of them are useful for understand the dynamics of granular flows.

In present study, a hybrid discrete-continuum model is developed for modeling the complex granular flow. The hybrid discrete-continuum model is aiming to have both the efficiency of the continuum model and the accuracy of the discrete model for the large scale hydrodynamics of granular flow. The basic idea of the method is to use the continuum method to describe large homogeneous region in the devices and use the discrete model to simulate the critical region where the continuum assumption breaks down. This kind of hybrid discrete-continuum model in present study is similar to the hybrid atomistic-continuum model for the micro- and nano-fluid flow[5, 6]. However, to the best of our knowledge, it is the first time to use it for modeling granular flow.

2. Method

In the continuum domain, the Navier-Stokes equation combined with kinetic theory of granular flow is applied to describe of the flow dynamics. And the discrete element method is used to describe the particle flows in the discrete domain. The mass and momentum conservation equations of continuum model are,

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{U}_s) = 0$$  \hspace{1cm} (1)
\[
\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s \mathbf{U}_c\right) + \nabla \cdot \left(\varepsilon_s \rho_s \mathbf{U}_c \mathbf{U}_c\right) = -\nabla p_s - \nabla \cdot \mathbf{t}_s
\]  
(2)

where \(p_s\) and \(\mathbf{t}_s\) are the granular pressure and solid shear tensor, respectively. The stress tensor is linearly related to the rate-of-strain tensor,

\[
\mathbf{t}_s = -\mu_s \left(\nabla \mathbf{U}_c + \nabla \mathbf{U}_c^\top\right) + \frac{2}{3} \mu_s \left(\nabla \cdot \mathbf{U}_c\right) \mathbf{I}
\]  
(3)

where \(\mu_s\) is shear viscosity. The particulate phase stresses are closed using kinetic theory of granular flows which solve a separate conservation equation for granular temperature \((\Theta_s)\) [7],

\[
\frac{3}{2} \left[ \frac{\partial \left(\varepsilon_s \rho_s \Theta_s\right)}{\partial t} + \nabla \cdot \left(\varepsilon_s \rho_s \mathbf{U}_c \Theta_s\right) \right] = (-\mathbf{p}_s \mathbf{I} + \mathbf{t}_s) : \nabla \mathbf{U}_c - \nabla \cdot \mathbf{q}_s - \gamma
\]  
(4)

The solids pressure and the solid viscosity are calculated according to Lun et al [8],

\[
p_s = \varepsilon_s \rho_s \frac{\Theta_s}{\Theta_{\text{max}}} + 2 \rho_s \left(1 + e\right) \varepsilon_s^2 g_0 \Theta_s
\]  
(5)

\[
\mu_s = \frac{4}{5} \rho_s d_p \varepsilon_s^2 g_0 \left(1 + e\right) \frac{\sqrt{\Theta_s}}{\pi} + \frac{\varepsilon_s \rho_s d_p \sqrt{\pi \Theta_s}}{6(3-e)} \left(1 + \frac{2}{5} \left(1 + e\right) \left(3e - 1\right) \varepsilon_s g_0\right)
\]  
(6)

\[
\lambda_s = \frac{4}{3} \varepsilon_s \rho_s d_p g_0 \left(1 + e\right) \frac{\sqrt{\Theta_s}}{\pi}
\]  
(7)

where the flux of fluctuating energy is closed using Fourier’s law of heat conduction,

\[
\mathbf{q}_s = -k_s \nabla \Theta_s
\]  
(8)

where the heat conductivity of granular phase is calculated as,

\[
k_s = \frac{150 \rho_s d_p \sqrt{\Theta_s \pi}}{384 (1 + e) g_0} \left[1 + \frac{6}{5} \varepsilon_s g_0 \left(1 + e\right) \right]^2 + 2 \rho_s \varepsilon_s^2 d_p \left(1 + e\right) g_0 \sqrt{\Theta_s \pi}
\]  
(9)

The collisional dissipation of granular energy is given as follows,

\[
\gamma = \frac{12 \left(1 - e^2\right) g_0}{d_p \sqrt{\pi}} \rho_s \varepsilon_s^3 \Theta_s^{3/2}
\]  
(10)

Within these formulations, \(g_0\) is the radial distribution function given as follows,

\[
g_0 = \left[1 - \left(\varepsilon_s \Theta_{\text{max}}\right)^{1/3}\right]^{-1}
\]  
(11)

The discrete element method originally developed by Cundall and Strack [4] is used in present study and the equation of motion solved for a particle is as follow,
The contact force is calculated based on linear spring-dashpot model. In this model, the normal component of the contact force between two particles is calculated as follow,

\[ F_{ab,n} = -k_n \delta_n n_{ab} - \eta_n u_{ab,n} \]  

where \( k_n \) is the normal spring stiffness, \( n_{ab} \) the normal unit vector, \( \eta_n \) the normal damping coefficient and \( u_{ab,n} \) the normal relative velocity. The overlap \( \delta_n \) is given by

\[ \delta_n = (R_a + R_b) - |r_b - r_a|, \]

where \( R_a \) and \( R_b \) denote the radii of the interacting particles, \( r_b \) and \( r_a \) denote the position vector of the particles.

The normal unit vector is defined as

\[ n_{ab} = \frac{r_b - r_a}{|r_b - r_a|} \]

The normal component of the relative velocity between particle \( a \) and particle \( b \) is

\[ u_{ab,n} = (u_{ab} \cdot n_{ab}) n_{ab} \]

The normal damping coefficient is calculated as follow,

\[ \eta_n = \frac{-2 \sqrt{m_{ab} k_n \ln e}}{\sqrt{\pi^2 + \ln^2 e}} \]

Equation (17) makes sure that the restitution coefficient \( (e) \) is same in both continuum model and discrete model.

Fig.1. shows a general schematic of the idea of the hybrid discrete-continuum model used in this work. The continuum model is used to solve the left part of the simulation domain, while the discrete particle model is applied to simulate the right part of the simulation domain. The interface between the two descriptions lies in \( y_2 \) as illustrated in Figure 1. The most important concern in the hybrid discrete-continuum model is to ensure the continuity of the physical quantities including the number of particles, the momentum and energy fluxes cross the interface. An overlapping region is constructed to couple these two different descriptions of granular flow. The overlapping region is solved by both two methods, therefore, the solution of the hydrodynamic variables are shared with each other. The \( y_1 \sim y_2 \) domain is the continuum model to particle boundary region where particles will be generated in this domain based on the flux of \( y_2 \) face calculated by continuum model. The number of particles to be inserted in a single continuum time step is given by,

\[ n = (A_i \cdot u_i) e_i \rho_e \Delta t_c / m_p \]  

where \( A_i \cdot u_i \) is the normal flux of the cell \( i \) and \( m_p \) is the mass of one particle. The new added particle will be random located in the interface provided that they do not overlap with the existed particles. Particle velocities are generated from a Maxwell distribution with mean and standard deviation determined by the local continuum velocity and granular temperature.

\[ f(r, u_p) = \frac{1}{(2\pi\Theta)^{3/2}} \exp \left[ -\frac{(u_p - u_e)^2}{2\Theta} \right] \]

Where \( u_e \) and \( \Theta \) is the average velocity and granular temperature calculated from the continuum model. Once a particle goes to the \( y_2 \sim y_3 \) domain, it will be deleted and contributed to the continuum model as follows,
\[ \varepsilon'_s = \varepsilon_s + \frac{V_p}{V_c} \]  

(20)

\[ \varepsilon'_s \mathbf{u}_c + \frac{V_p \mathbf{u}_p}{V_c} \]

\[ \mathbf{u}_c = \frac{\varepsilon'_s}{\varepsilon_s} \]  

(21)

Where \( V_p \) and \( V_c \) is the volume of one particle and the computational cell, \( \mathbf{u}_p \) is the deleted particle’s velocity.

Fig. 1. Schematic of the basic idea of the hybrid discrete-continuum model

Fig. 2. shows the typical flag matrix used in the hybrid discrete-continuum model. Each computational cell is assigned a number to represent the type of the cell. For the pure continuum model region, the flag of the cell is set to 0. For the pure discrete particle region, the flag of the cell is set to 3. Particles will be added in the cell with the flag equated to 2 and deleted in the cell with the flag equated to 1.

Fig. 2. Flag matrix of the hybrid discrete-continuum model

3. Results

To demonstrate the feasibility of the proposed hybrid discrete-continuum model, we consider an example of a velocity-driven granular Poiseuille flow. The particles flowing in a channel without gravity are assumed to be mono-disperse and smooth (frictionless). The problems are simulated using all the three methods, i.e. the continuum model,
the discrete model and the hybrid model. In this case, the particles are inserted into the channel continuously with equal velocity. Fig.3. shows the mass of the particle predicted by all the three models, it can be seen that all the three models predicted the same trend and the same quantitative value when the flow reach a steady state in the channel, this indicates the excellent consistency of the three methods with respect to mass conservation. Fig.4. shows the radial solid velocity and solid volume fraction predicted by all the three models at the middle of the channel, all the three models predicted a homogenous solid volume fraction and solid velocity, which indicated that the mass and momentum are conserved in the present hybrid model, and more importantly, the idea has been correctly implemented and validated.

![Fig.3. The mass of particle in the channel predicted by different models](image)

![Fig.4. The radial solid velocity and solid volume fraction predicted by different models (at the middle of the channel)](image)

**4. Conclusion**

In present study, we have developed a hybrid discrete-continuum model for complex granular flow. A velocity-driven granular Poiseuille flow is simulated to show the feasibility of the idea of hybrid discrete-continuum model and demonstrate the correctness of implementation. In perspective, the Navier-Stokes equation combined with the kinetic theory of granular flow can be applied to describe of the flow dynamics where continuum assumption is validated and the discrete element method is used to simulate the critical region where the continuum assumption breaks down. The hybrid discrete-continuum model is therefore expected to take the advantages of the efficiency of continuum model and the accuracy of discrete model, when modeling large scale hydrodynamics of granular flow.

**References**