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Discrete element simulation of particle flow in arbitrarily complex geometries

Junwei Su [a,d], Zhaolin Gu [b,c,*], Xiao Yun Xu [d,**]

[a] School of Mechanical Engineering, Xi'an Jiaotong University, Xi'an 710049, China
[b] School of Human Settlements and Civil Engineering, Xi'an Jiaotong University, Xi'an 710049, China
[c] SKLLQG, Institute of Earth Environment, Chinese Academy of Sciences, China
[d] Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK

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ABSTRACT

Conventional simulations of dense particle flows in complex geometries usually involve the use of glued particles to approximate geometric surface. This study is concerned with the development of a robust and accurate algorithm for detecting the interaction between a spherical particle and an arbitrarily complex geometric surface in the framework of soft-sphere discrete element model (DEM) without introducing any assumptions. Numerical experiments specially designed to validate the algorithm shows that the new algorithm can accurately predict the contact state of a particle with a complex geometric surface. Based on the proposed algorithm, a new solver for simulation of dense particle flows is developed and implemented into an open source computational fluid dynamics (CFD) software package OpenFOAM. The solver is firstly employed to simulate hydrodynamics in a bubble fluidized bed. Numerical results show that a 3D simulation can predict the bubble size better than a 2D simulation. Subsequently, gas–solid hydrodynamics in an immersed tube fluidized bed is simulated. Results show that bubble coalescence and breakup behavior around the immersed tubes are well captured by the numerical model. In addition, seven different particle flow patterns around the immersed tubes are identified based on the numerical results obtained.

1. Introduction

Multiphase particle systems are extremely common in nature and industry. Detailed knowledge of the flow behaviors of particle cloud is important for scientific research and industrial applications. Numerical modeling can provide more detailed information about the system characteristics. Thus, in the last two decades significant research efforts have been devoted to the development of numerical models to study the complex hydrodynamics of dense particle flows, including gas–solid flows in fluidized bed (Ding and Gidaspow, 1990; Gidaspow, 1994; Hoomans et al., 1996; Tsuji et al., 1992; Xu and Yu, 1997) and bubble flows in bubble column reactors (Delnoij et al., 1997; Sokolichin and Eigenberger, 1999; Sokolichin et al., 1997). All these models can be broadly categorized into Eulerian methods and Lagrangian methods. In Eulerian methods, both particle and fluid phases are continuous and fully interpenetrating. Eulerian methods can predict the overall behaviors of a system with relatively low computational cost. A commonly and widely used Eulerian model is the two-fluid model (TFM), in which mass and momentum conservation equations are solved for each phase. This model has been widely used to simulate various fluidized bed systems (Boemer et al., 1997; Mathiesen et al., 2000; Samuelsberg and Hjertager, 1996). However, due to the continuum description of the dispersed system, TFM has to incorporate additional closure relations for particle–particle interaction by using either empirical formulae (Gidaspow et al., 1983) or kinetic theory of particle flow (Deen et al., 2001; Pfleger et al., 1999; Sokolichin and Eigenberger, 1999). Moreover, additional closure models for mass exchange or inter-phase interaction are also needed if necessary.

Eulerian methods can provide macroscopic characteristics of a multiphase system, which is helpful in gaining a broad understanding of a particulate process of interest. However, macroscopic behaviors of a particulate matter are controlled by interactions between individual particles as well as interactions between particles and their surrounding fluids and walls. Understanding the microscopic mechanism in terms of these interactions is, therefore, the key leading to truly interdisciplinary research into particle matter and producing results that can be generally used (Zhu et al., 2007). Discrete element method (DEM)

* Corresponding author at: School of Human Settlements and Civil Engineering, Xi'an Jiaotong University, Xi'an 710049, China.
** Corresponding author.
E-mail addresses: guzhaoln@mail.xjtu.edu.cn (Z. Gu), yun.xu@imperial.ac.uk (X.Yu. Xu).

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as a Lagrangian method is widely used in particle flow simulations to offer more microscopic information, such as trajectories of individual particles and transient forces acting on individual particles, which is difficult, even impossible to obtain by other macroscopic models or experiments (Zhu et al., 2007).

Two types of DEM, the hard-sphere model (Hoomans et al., 1996) and the soft-sphere model (Cundall and Strack, 1979), have been developed. In the hard-sphere model, a sequence of collisions are processed instantaneously one after another, but the forces between particles are not explicitly considered. The hard-sphere DEM model is more suitable for simulations of dilute or rapid granular flows since it considers two-body collisions only. It has also been used to simulate dense particle flows in complex geometries (Gui and Fan, 2009; Wu et al., 2009, 2006), owing to its ability to accommodate arbitrary geometry. However, at high particle number densities or low coefficients of normal restitution, collisions in a hard-sphere model may lead to a dramatic reduction in kinetic energy. This is the so-called inelastic collapse (Mcnamara and Young, 1992), in which regime the collision frequencies diverge as relative velocities become infinitely small. In such a case, the hard-sphere method would fail and new methods need to be sought (Deen et al., 2007). In the soft-sphere model, the inter-particle contact forces, namely, the normal, damping and sliding forces, are computed using equivalent simple mechanical elements, such as springs, dash dots and sliders. The motions of particles are described by the well-established Newton's second law. The soft-sphere model is preferable for numerical simulations of dense particle flows since it incorporates multiple particle–particle contacts which are important in dense particle systems, especially in quasi-static systems. Moreover, non-contact force can also be incorporated into soft sphere model easily. Detailed reviews of the theoretical development of DEM and its applications can be found in Zhu et al. (2007, 2008).

Although the soft-sphere DEM model has received considerable attentions, most of its applications are limited to particle flows in relatively simple geometries owing to the difficulty in tracking particle motion in an arbitrary, unstructured mesh and the difficulty in detecting the interaction between a particle and a complex geometry surface, especially in 3D.

A recent study by Macpherson et al. (2009) has provided a feasible solution to the first challenge. This algorithm has been implemented into open source C++ toolbox OpenFOAM (OpenCFD, 2011b) as a basic library for Lagrangian tracking and is ready to use. OpenFOAM is a C++ toolbox based on object oriented programming (Weller et al., 1998) designed for continuum mechanics applications, specially CFD applications. Within the OpenFOAM framework, one can customize solvers or extend the numerical libraries to their own needs relatively easily which is a major advantage over commercial software. There is an increasing number of researchers who are using OpenFOAM as their developing platform in their work (Bannari et al., 2011; Favero et al., 2010; Selma et al., 2010; Silva et al., 2008).

The second difficulty has been tackled by Kremmer and Favier (2001) who proposed a finite wall method for detecting particle–wall collision and introduced a shrink factor to eliminate multiple calculations of contact force due to overlapping. However, the value for the shrink factor is case or user experience dependent. Moreover, this method can only be used with a triangular boundary mesh, limiting its usage, especially when coupled with CFD calculations. Traditionally, glued spheres are used to represent the surface of a complex geometry (Kodam et al., 2009) so that detection of interaction between a particle and complex geometry surface is carried out in exactly the same way as that of particle–particle interaction. However, this method requires additional effort for particle configuration of a complex geometry. Moreover, convex points or lateral edges of the geometry cannot be accurately represented and different particle configurations may result in different particle behaviors.

In order to overcome the aforementioned difficulties associated with the detection of particle–surface interactions in a soft-sphere DEM model, a new algorithm, namely **RIGID** (**s**phe**R**ical part**I**cle and **G**eometry **I**nteraction **D**etection), has been developed for the detection of interactions between a spherical particle and an arbitrarily shaped rigid wall surface in the soft-sphere model framework without introducing any assumption. In the next section, mathematical models for the continuous phase and soft-sphere discrete element are described. The novel detection algorithm for the interaction between spherical particles and arbitrarily shaped surface is described in Section 3. An elaborate numerical experiment to test the algorithm together with comparisons of efficiency and accuracy between **RIGID** and the traditional glued particle method are presented in the first part of Section 4, followed by two further test cases, i.e. bubble fluidized bed and an immersed tube fluidized bed aiming to test **RIGID** for dense particle flows. Finally, conclusions are drawn and possibilities of further development of the current algorithm are discussed.

In summary, this work focuses on developing an algorithm, namely **RIGID,** for detecting particle interactions with an arbitrarily complex wall in the framework of soft-sphere model and applying it to simulations of dense gas–particle flows in complex geometries. By using this algorithm, the applicability of DEM to industrial problems may be significantly improved.

2. Mathematical models

2.1. Continuous phase hydrodynamics

The continuous phase model for dense particle flows can be written as follows (Xu and Yu, 1997):

$$\frac{\partial \varepsilon}{\partial t}+\nabla\cdot(\varepsilon\mathbf{u})=0 \tag{1}$$

and

$$\frac{\partial(\rho_f\varepsilon\mathbf{u})}{\partial t}+\nabla\cdot(\rho_f\varepsilon\mathrm{uu})=-\varepsilon\nabla p-\mathbf{F}^{f-p}+\nabla\cdot(\varepsilon\Gamma)+\rho_f\varepsilon\mathbf{g} \tag{2}$$

where ρ_f, ε and $\mathbf{u}$ are the density, volume fraction and velocity of the continuous phase, respectively; p is the pressure, Γ is the viscous stress tensor, and $\mathbf{F}^{f-p}$ is the volumetric fluid–particle interaction force, which can be drag force, pressure gradient force, Basset force, or Magnus force. In a gas–solid system, drag force and pressure gradient force are usually considered. The Ergun/Wen and Yu drag model is adopted in this work, its exact expression along with the pressure gradient force can be found in Bokkers et al. (2004). It should be pointed out that when evaluating the volume fraction ε and volumetric fluid–particle interaction force $\mathbf{F}^{f-p}$, the cell in which a given particle resides should be determined first. In this work, the particle tracking model of Macpherson et al. (2009) in unstructured, arbitrary polyhedral meshes implemented in OpenFOAM (OpenCFD, 2011b) is adopted.

2.2. Soft sphere model

According to Cundall and Strack (1979), the normal component of the contact force, $\mathbf{F}_{nij}^{p-p}$, acting on particle i by particle j (or wall) (particles i and j are two interacting spherical particles), is obtained as the sum of the spring and dash–dot forces, i.e. $\mathbf{F}_{nij}^{p-p}$ for