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A novel two-grid formulation for fluid–particle systems using the discrete element method

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ABSTRACT

Discrete element modeling (DEM) coupled with computational fluid dynamics (CFD) provides an excellent platform to analyze fluid–particle systems. In all previous work, the fluid and particle systems are solved on a single grid. Contradictory requirements posed by resolution of fine scale fluid features such as turbulence, friction and heat transfer coefficient at immersed surfaces, and the resolution of important geometrical features, versus the necessity to maintain smoothness in particle solid fraction distribution on the chosen grid, often make single grid calculations untenable. To overcome this challenge, we have developed a novel two-grid technique in which a coarser particle grid is mapped on to a fine fluid grid. The technique uses suitable mappings to transfer fluid field variables from fluid-to-particle grid, and interphase transfer terms and void fractions from particle-to-fluid grid. The method is applied to a jetting fluidized bed of 750 μm particles with a characteristic jet width of 1.6 mm. Results in the form of time-averaged void fractions and solid-velocity for two inlet jet velocities with single and multiple jets are compared to experiments. The results agree reasonably well with the experiments validating the two-grid approach for cases where single grid DEM–CFD would have been difficult to apply.

1. Introduction

Recent advances in computational power enable us to perform high fidelity numerical simulations on granular flows. Discrete element modeling (DEM) and two-fluid-model (TFM) are the two most widely used numerical methodologies for modeling granular flows like fluidized beds and spouted beds. The two methods differ fundamentally in the approach they follow. DEM is an Eulerian–Lagrangian approach where the fluid flow is solved in an Eulerian framework while tracking each individual particle in a Lagrangian fashion. On the other hand, TFM considers the gas and solid to be two interpenetrating media and solves for their interaction in an Eulerian–Eulerian approach. DEM provides higher resolution compared to TFM as it resolves the complete dynamics of each particle in the flow. Additional closure equations are required in TFM to account for the continuum description of particles. No such closure laws are required in DEM as it treats the particles individually. DEM was first developed by [1] and later adopted for simulation of fluidized beds and coupled with CFD by [2]. Since then, DEM has been used in investigating a wide variety of applications including surface diffusion problems [3,4], modeling behavior of cohesive particles [5,6], segregation of binary particle mixtures [7,8], capturing bubble dynamics in fluidized beds [9–11] and so on. A comprehensive review focusing on the research work done using DEM has been given by [12–14]. Two broad categories of discrete particle methods (DPM) are available for modeling fluid–particle interactions namely resolved and unresolved, respectively. A resolved discrete particle model (RDPM) is much like a direct numerical simulation (DNS), where fluid boundary conditions are prescribed on the boundary of each individual particle. Arbitrary Lagrangian Eulerian (ALE) and immersed boundary method (IBM) are two of the most popular techniques used to specify the no-slip boundary conditions on the particle surface for RDPM. RDPM is generally used to model flows at very small scales, without the requirement of fluid drag closures on the particle surface. The unresolved DPM (UDPM) on the other hand does not require fluid boundary conditions to be specified on the particle surface as they use drag closure equations. UDPM's have become popular due to their ability to predict fluid–particle interactions with considerable accuracy without the need to have sophisticated grid resolution techniques near particle surfaces. A detailed review on the different numerical techniques adapted to model gas–solid flows at different scales has been given by [15].

Till now mostly a single-grid approach has been used for DEM–CFD calculations, i.e., the particle and fluid calculations are done on the same grid. This has an inherent problem in that the resolution requirements for the particle and fluid fields are contradictory to each other. Generally, fine grids are required to resolve the fluid flow field. Fine grids for flow resolution become particularly important to resolve small geometrical features which influence the flow, when the interstitial flow is turbulent, and when velocity and temperature gradients need to be resolved at surfaces for calculating wall shear stresses and heat transfer coefficients. The fine fluid grids however, conflict with particle field resolution requirements which require that the grid size

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should be large enough to represent the local volume fraction of the particulate phase properly [16]. Too few particles in a cell result in sharp changes of the solid fraction field across cells whenever particles cross cell boundaries. This can lead to large spatial and temporal fluctuations in the fluid volume fraction across cells ultimately making the numerical integration unstable.

This aspect has been worked on in the literature by [17,18] who performed a combined experimental and computational study to find flow regimes in a spouted fluidized bed using a DEM–CFD methodology. In their method performed on a single grid finer than the particle diameter, they have represented each individual particle within a porous cube halo of predetermined size which moves with the particle. The solid fraction representing the particle is spread over the porous cube and then distributed over the finer fluid cells in a volume weighted manner. This is done for all particles. In doing so, they prevent numerical instabilities arising due to the presence of finer fluid cells in comparison to particle size by smoothing out the variation in solid fraction. The porous cube halos can intercept a fluid cell in any possible fashion which requires a calculation of the fraction of the finer cells being intercepted by the porous cube. For a 3D simulation having millions of particles, the calculation of this cell fraction at every time step can be computationally expensive. The other difficulty arising out of the porous cube method is the communication overhead across interblock/interprocessor boundaries, needed for parallelization, where information regarding these fraction of cells intercepted need to be communicated between processors. Depending on the position of a particle near an interprocessor boundary, varying volumes of the porous cube could be present on a neighboring processor. This scenario would necessitate determining the number of cells influenced by the porous cube on the adjoining processor for each particle in the vicinity of the boundary, followed by packing and communication. This can cause inefficient parallelization and thus severely limit the parallel scalability.

In this work, we have developed a two-grid formulation for systems involving DEM–CFD coupling in a parallel processing framework. In this formulation, the fluid flow equations are solved on a fine grid which is independent of the particle size, whereas the discrete particle equations are solved on a coarser grid in which each coarse particle cell is composed of multiple fluid cells. Recently, a similar technique has been used by [19] to conduct 2D Lagrangian modeling of fuel mixing in fluidized beds. The approach that they have used is similar to what we independently propose in our present work. One important difference lies in the way the void fractions are calculated in each of the fluid cells. In their work, the exact void fractions are calculated based on the volume of particles intercepted at each fluid cell. This is time-consuming, and extremely complicated for a three-dimensional fluid–particle coupled problem involving thousands of particles. To avoid this, we calculate the void fractions at the particle cell and map the same value back to each of the fluid cells that fall within that particular particle cell. This present approach might result in small inaccuracies, but for a domain having tens of thousands of particles; the inaccuracies would be negligible compared to the ease and swiftness of the simulations.

The new scheme is tested in a jetting fluidized bed and the results have been validated with experiments [20] performed on the same geometry. Relatively large, 750 μm particles have been used for the tests. Single, double and triple jet configurations have been studied using the new two-grid formulation. Each jet is of size 1.6×4.95 mm^2. Using a single grid is not possible for the large particle size of 750 μm as the requirement of having 3–4 particles in each direction of a fluid cell [21] is not satisfied. In the single grid formulation, the grid size at the jet entrance plane should be equal to the jets or smaller than it. But in the case of 750 μm particles and 1.6 mm jet width, even the largest possible grid size using a single grid cannot satisfy the discrete phase requirement of having a smooth void fraction. The two-grid formulation overcomes this limitation by allowing the jets to be resolved on the fluid grid as well as satisfying the requirements of a smooth void fraction on the particle grid. The method proposed in this paper avoids the complications of the porous cube method by considering two separate fixed grid definitions, which intercept each other in a regular pattern thus facilitating inter-processor communications. The calculation overhead of calculating a very high number of cell fractions is also not required in this method thus aiding in simpler and faster calculations, needed for a large number of particles in three-dimensions. The paper is structured as follows. The next section describes the methodology used in the single-grid and two-grid DEM followed by a section on results and discussion, and the conclusions.

2. Methodology

Discrete element modeling (DEM) coupled with CFD code GenIDLEST [22,23] (Generalized Incompressible Direct and Large Eddy Simulation of Turbulence) has been used to numerically model the particle–fluid interactions in a jetting fluidized bed. DEM offers two different approaches for resolving the particle–particle collisions. They are the hard sphere [24] and soft sphere [1] approaches respectively. In our analysis, the soft sphere approach is considered as it allows for multiple particle interaction which is predominant in dense fluidized beds unlike the hard sphere technique which can account for binary collisions only. Both the fluid solver and DEM are parallelized for use with multiprocessor systems [25,26].

2.1. Particle governing equations

The motion of each particle is tracked based on Newton's Law of motion as follows:

$$m_p \frac{d\vec{v}_p}{dt} = V_p\left(\rho_p - \rho_g\right)\vec{g} + \vec{F}_{p,Drag} + \vec{F}_{p,Collision} \tag{1}$$

$$I_p \frac{d\vec{\omega}_p}{dt} = \vec{T}_{p,Collision} \tag{2}$$

where $m_p, \vec{v}_p, V_p, \vec{F}_{p,Collision}$ are the particle mass, velocity, volume, and collision forces, respectively. $I_p, \vec{\omega}_p, \vec{T}_{p,Collision}$ represent particle moment of inertia, particle rotational velocity, and total torque acting on the particle, respectively. Integrating Eq. (1) in time advances the linear position of the particle whereas integrating Eq. (2) updates the angular motion of the particle at each time step.

2.1.1. Particle–particle collision formulation

The soft sphere model handles particle–particle collisions as finite particle overlaps. Fig. 2 shows the entire mechanism. Using the overlap, the inter-particle forces are calculated based on a linear spring analogy in the normal and tangential directions respectively. An additional dashpot arrangement is present in parallel to the springs. The deflection of the particles after a collision is governed by the spring, whereas the inelasticity of collisions is taken care by a damper through energy dissipation. An additional sliding element is placed in series with the spring mass damper in the tangential direction. The slider allows the particles to slide against each other as well, limiting the maximum magnitude of the tangential force. Spring constants and damping coefficients in the normal and tangential directions are used to calculate the normal and tangential forces respectively due to the particle overlaps. The following equations are used for the inter-particle collisions. The equations deal with the motion of particle p when it collides with particle q.

$$\vec{f}_{n,pq} = -k_n \vec{\delta}_{n,pq} - \eta_n \vec{v}_{n,pq} \tag{3}$$

$$\vec{f}_{t,pq} = -k_t \vec{\delta}_{t,pq} - \eta_t \vec{v}_{t,pq} \tag{4}$$

where $\vec{f}_{n,pq}, \vec{f}_{t,pq}, k_n, k_t$ are the normal force, tangential force,