Journal of Computational Physics 243 (2013) 109–129

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A variable-density fictitious domain method for particulate flows with broad range of particle–fluid density ratios

Sourabh V. Apte *, Justin R. Finn

School of Mechanical, Industrial, and Manufacturing Engineering, Oregon State University, Corvallis, OR 97331, United States

ARTICLE INFO

Article history:
Received 4 August 2012
Received in revised form 20 December 2012
Accepted 21 December 2012
Available online 7 February 2013

Keywords:
Fully resolved simulations
Fictitious domain method
Particulate flows
High-density ratio
Particle–vortex interactions

ABSTRACT

A numerical scheme for fully resolved simulation of particle–fluid systems with freely moving rigid particles is developed. The approach is based on a fictitious domain method wherein the entire particle–fluid domain is assumed to be an incompressible fluid but with variable density. The flow inside the particle domain is constrained to be a rigid body motion using an additional rigidity constraint in a fractional step scheme. The rigidity constraint force is obtained based on the fast computation technique proposed by Sharma and Patankar (2005) [1]. The particle is assumed to be made up of material points moving on a fixed background mesh where the fluid flow equations are solved. The basic finite-volume solver is based on a co-located grid incompressible but variable density flow. The incompressibility constraint is imposed by solving a variable-coefficient pressure equation. Use of density-weighted reconstruction of the pressure gradients was found to give a stable scheme for high density ratio particle–fluid systems. Various verification and validation test cases on fixed and freely moving particles are performed to show that the numerical approach is accurate and stable for a wide range (10^{-3}–10^{6}) of particle–fluid density ratios.

1. Introduction

Fully resolved simulations (FRS) of particle–fluid systems, wherein all scales associated with the fluid and particle dynamics are completely captured from first principles, are of great importance for understanding disperse particulate flows with applications in environmental engineering, biological flows, chemical reactors, and energy conversion systems; for example, sediment transport, aeolian transport, red blood cells, coal-particle combustors, bubbly flows in fluidized beds, catalytic reactors, among others. Many of these applications involve complex configurations and unsteady, often turbulent flows and their fundamental understanding is of critical importance. Such direct numerical simulation techniques are useful to obtain detailed data that can be used to develop subgrid and reduced order models used in other approaches for particulate flows such as Euler–Lagrange discrete element modeling, wherein the disperse particle dynamics is modeled through closure laws for drag, lift, added mass and other forces exerted by the fluid.

Several numerical schemes have been developed for fully resolved simulations of *freely moving, rigid particles* in a fluid flow. These can be categorized as (i) body-fitted, (ii) mesh-free, and (iii) fixed-grid methods. The body-fitted grid approach, such as boundary element [2] and arbitrary Lagrangian–Eulerian (ALE)-based finite-element approach on unstructured grids [3] method, use moving grids that conform to the shape of the immersed particles. Moving mesh algorithm based on space-time finite-element approach was also developed by Johnson and Tezduyar [4] to calculate falling particles in a tube. Such approaches provide an accurate solution at the particle–fluid interface, but suffer from the complexity of the moving mesh

* Corresponding author. Tel.: +1 541 737 7335; fax: +1 541 737 2600.
E-mail address: sva@engr.orst.edu (S.V. Apte).

0021-9991/$ - see front matter
http://dx.doi.org/10.1016/j.jcp.2012.12.021

and regeneration algorithms. Use of these techniques in three-dimensions significantly increase the computational cost and memory requirements. Smoothed particle hydrodynamics (SPH) is a *mesh-free* technique commonly used for multiphase flows with free-surfaces [5]. Fixed grid approaches, such as distributed Lagrange multiplier and fictitious-domain methods, immersed boundary method, lattice Boltzmann method, among others, are most popular for such simulations owing to their simplicity in computing motion of arbitrary shaped objects.

Considerable work has been done on fully resolved simulations of freely moving particles in fluid flows on fixed grids. For example, distributed Lagrange multiplier/fictious domain (DLM) based methods [6] and immersed boundary method (IBM by [7–11]) have been developed and shown to be very effective in computing particle–fluid systems and fluid–structure interaction problems. Lattice Boltzmann method (LBM by [12]) has been developed and effectively used for simulations of rigid as well as deforming particles. Combination of the DLM, direct forcing based IBM, and Lattice–Boltzmann method (termed as *Proteus*) was recently developed [13]. A second-order accurate fixed grid method (PHYSALIS) has also been proposed [14], which gives good solutions for *spherical* particles by using local spectral representations of the solution near a spherical boundary.

The immersed boundary method has traditionally been used for fluid–structure interaction problems with the motion of the immersed object specified (stationary, forced rigid motion, or elastically deforming objects). For such applications, two different implementations are typically used involving 'direct continuous forcing' wherein a continuous forcing function around the particle boundary is added to the Navier–Stokes equations [7,15,16] or 'discrete forcing' wherein forcing is either explicitly or implicitly applied to the discrete equations [17–20,10,11]. The former is a straightforward approach that can be implemented in any Navier–Stokes solver with relative ease, however, diffuses the interface boundary proportional to the grid spacing owing to interpolation functions. The latter allows precise satisfaction of the boundary condition at the immersed surface maintaining a sharp interface representation, however, its implementation for arbitrary shaped objects can become fairly involved. Recently, Kim and Choi [10] developed a new immersed boundary method using the conservative form of Navier–Stokes and continuity equations in the non-inertial frame of reference and applied to fluid–structure interactions problems with the motion of the immersed objects specified (forced) or predicted as for freely moving rigid particles. With sufficient grid resolutions, both approaches have been shown to provide grid-convergent and accurate results.

For freely moving particle-laden flows, use of relatively coarse grids near the interface is necessary especially if the approach is used to study large number of particles (on the order of 1000) in complex flows. In such flows, use of grid resolution with more than 20–25 grid points per particle can become prohibitively expensive. Direct forcing techniques may result in large oscillations in the forces exerted by the fluid on the particle if the particle moves in such a way that the local stencil near the boundary changes abruptly. This, although not an issue for specified motion fluid–structure interaction problems, can cause problems to freely moving particulate flow problems. It is especially important for simulations with relatively coarse resolution of the interface between the particle and the fluid. Continuous forcing immersed boundary approaches on the other hand do not seem to show such an issue as the forces are regularized prior to discretization [9]. The relative ease of implementation for continuous forcing methods makes them attractive for freely moving large number of disperse particles in complex turbulent flows. However, the numerical approach by Uhlmann [9] has been found to be stable only for particle-to-fluid density ratio ($\rho_P/\rho_F > 1$) and has only been used for density ratios up to 10, whereas for particle-air systems the density ratios can easily range on the order of 10^3. For lighter than fluid particles or neutrally buoyant particles, the scheme has been found to become unstable. Recently, Kempe and Frohlich [21] suggested modifications to the approach that increased the range of applicability of the method to lighter than fluid particles and tested the scheme for $0.3 < \rho_P/\rho_F < 10$.

Taira and Colonius [22] proposed a new implementation of the immersed boundary method to achieve second-order accuracy. They compared IBM with fictitious-domain based methods to point out subtle differences when the immersed objects are constrained to undergo specified motion. In the fictitious domain/DLM method (see [6,23]), the entire fluid–particle domain is assumed to be a fluid and the flow inside the entire particle domain is constrained to be a rigid-body motion through rigidity constraint in terms of a stress or a force. The rigidity constraint force is applied over the entire particle domain as opposed to the continuous forcing immersed boundary method of Uhlmann [9] where the forcing function is present very close to the interface, giving rise to fluid-like flowfield inside the particle region. Sharma & Patankar [1] proposed a fast technique to obtain the rigidity constraint force that eliminated the need for an iterative procedure to solve for the rigid body motion in laminar flows. Recently, Veeramani et al. [24] proposed a similar approach in the context of finite-element methods and used constant fluid density even within the particle domain. Apte et al. [25] further developed the finite-volume based fictitious domain approach by [1] to large number of particles in complex turbulent flows on co-located grids and improved the temporal and spatial accuracy. Their approach [25] uses the true local density at a control volume, equal to the fluid in the fluid region and equal to the particle in the particle region, and constant coefficient Poisson solvers based on multigrid approaches for fast convergence. This approach does not suffer the stability issue as in Uhlmann [9] and has been used for particle-to-fluid density ratios over the range of 0.1-20.

All of the above approaches have only been applied to particle–fluid systems with relatively low range of density ratios between the two-phases ($\mathcal{O}[10^{-1} - 10]$). Large density ratios are common in many practical applications involving complex flows; for example coal particles in a oxycoal boiler, aeolian particle transport, aerosol transport, microfluidics, among others. Sharp gradients in density across the particle–fluid interface in turbulent flows, for example in *gas–solid* systems such as aeolian transport, chemical reactors ($\mathcal{O}[10^3]$) or lighter than fluid solid–liquid or bubbly flow systems, can cause numerical 'ringing' of the solution and lead to numerical instabilities when using the fictitious domain approach with fast computation of the rigidity constraint [1,25]. In the present work, we extend this numerical approach to account for particle–fluid systems