Journal of Computational Physics 230 (2011) 1749–1765

Contents lists available at ScienceDirect

Journal of Computational Physics

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

A pressure boundary integral method for direct fluid–particle simulations on Cartesian grids

Julian A. Simeonov *, Joseph Calantoni

Marine Geosciences Division, Naval Research Laboratory, Code 7434, Bldg. 1005, Stennis Space Center, MS 39529, USA

ARTICLE INFO

Article history:
Received 20 February 2010
Received in revised form 24 September 2010
Accepted 16 November 2010
Available online 2 December 2010

Keywords:
Particle-laden flow
Direct numerical simulations
Discontinuous pressure Poisson equation
Boundary integral method

ABSTRACT

We consider a new Cartesian grid method for direct numerical simulations of fully coupled interaction of incompressible flow and spherical particles, based on a discontinuous extension of the pressure Poisson equation (PPE) across particle boundaries. We give a complete mathematical description of the boundary-integral treatment of the discontinuous PPE that includes the derivation of a new pressure boundary condition for accelerating boundaries and the solution of the system of boundary integral equations using spherical harmonics expansions. The model was validated with the standard test for finite Reynolds number flow around a sphere and with a novel test using the analytical solution for the Stokes flow past two adjacent spheres moving with the same velocity. The model capability and numerical efficiency was demonstrated with simulations for the collective settling of groups of 64–512 particles.

Published by Elsevier Inc.

1. Introduction

We consider a numerical modeling framework for finite Reynolds number particle-laden flows where the fluid phase is resolved at sub-particle scales through direct solution of the Navier–Stokes equations. The hydrodynamic forces acting on the particles are then computed by integration of the resolved pressure and viscous stresses over the particle surface. Resolving the boundary layers at the particle surface is usually achieved by using boundary-fitting grids with a grid step that decreases towards the boundary (e.g., [13]). While this technique is optimal for single particle simulations the evolving geometry in simulations with a large number of mobile particles requires frequent mesh re-generation [10]. 3D fluid–particle simulations requiring a minimal frequency of remeshing may be achieved using state-of-the-art moving mesh techniques [14]. For the purpose of such large-scale simulations, our goal here is to develop an inexpensive hydrodynamic solver based on fixed Cartesian grids that gives acceptable predictions for the hydrodynamic particle forces with a minimum number of grid points per particle diameter. Such solvers have demonstrated recently (e.g., [23]) that flows around spheres for particle Reynolds numbers in the range $10 < Re < 100$ can be modeled with as little as 16–32 grid points per diameter. Similarly, our focus here will be on the performance and the fidelity of the proposed numerical scheme at such low resolutions and low Reynolds numbers. The work is motivated by marine sediment transport applications where the particle Reynolds number seldom exceeds a few hundred.

The pressure field is the main difficulty in solving the incompressible Navier–Stokes equations in a domain with moving particle boundaries because the motion of each particle is felt instantaneously through the entire pressure field and the remaining particles. Our approach to solve this complicated *N*-body pressure problem belongs to a group of fictitious domain/Cartesian grid methods where the boundary value problem (BVP) is simplified by including particle interiors in

* Corresponding author. Tel.: +1 228 688 4206; fax: +1 228 688 4853.
E-mail address: simeonov@nrlssc.navy.mil (J.A. Simeonov).

0021-9991/$ - see front matter Published by Elsevier Inc.
doi:10.1016/j.jcp.2010.11.027

an extended model domain and modifying the equations using some device that represents the effect of the removed boundary. The modified equations can then be solved on a uniform Cartesian grid but the price for this computational advantage is that one has to deal with discontinuous solutions. In the immersed boundary method of Peskin [20] for incompressible flows interacting with elastic membranes, the boundary moves with the local velocity and exerts a singular force on the fluid. Similarly, in the virtual boundary method [7] the effect of boundaries is modeled as a drag force distributed on the boundary surface and proportional to the local fluid velocity. The ad hoc force is added to the Navier–Stokes equations and the latter are solved over the entire domain, including the particle interior. In both Peskin [20] and Goldstein et al. [7] the first order spatial discretization of the singular force results in overly smoothed solution discontinuities. Furthermore, the actual fluid surface force is not known in advance but must be obtained as part of the solution and generally depends on the far field flow conditions. Another fictitious domain method is the distributed Lagrange multiplier method [6] where a fictitious stress is added in order to maintain the interior fluid in solid body rotation. The unknown stresses are obtained as part of the solution of a weak variational formulation of the combined fluid–particle momentum equation that permits certain solution discontinuities.

Green function methods can also be used if the Navier–Stokes equations are "linearized" by treating the non-linear advection as a given source term in the momentum equation [3]. The resulting Stokes-like linear PDEs for velocity and pressure have discontinuities across particle boundaries in the form of single and/or double layer potentials [5] that must be determined by solving boundary integral equations. In electrostatic potential applications, such boundary integral equations are usually solved with the boundary element method [17] and an accelerating scheme such as the fast multipole method [9]. Our boundary integral method differs in several important aspects. First, while we do extend the pressure solution across particle boundaries, the momentum equation is solved solely outside the particles; updating the velocity field with explicit time integration is then straightforward once the pressure field is known. The solution of the discontinuous Poisson equation for pressure is sought in terms of a single layer potential with a continuous pressure and a discontinuous pressure gradient across the boundary. Second, we solve the pressure boundary integral equation by expanding the unknown surface density of the single layer potential in surface spherical harmonics rather than Boundary Element interpolating functions. The expansion reduces the boundary integral equation to a diagonally dominant linear system for the harmonic coefficients, which is solved with Gauss–Seidel iterations. Once the single layer density is determined, the pressure at every point can be computed by evaluating the single layer potential integrals. We use a more efficient method proposed by Mayo [18] where the *computed* pressure discontinuities are used to correct the finite-difference approximation of the Laplacian for finite-difference stencils crossing the boundary. The resulting regularized discrete Poisson equation for pressure can then be solved very efficiently with fast Poisson solvers. The computational advantage of such fast Poisson solvers is the main motivation for the present fictitious domain approach based on Cartesian grids.

The emphasis here is on the boundary integral method for the pressure. Thus, the numerical treatment of the momentum equation is kept as simple as possible and is based on simple second order finite-differences. An important desirable aspect in the modeling of particle-laden flows is the ability to simulate the close hydrodynamic interaction of particles. In this paper, we compare our numerical solution for a "rigid pair" of spheres falling parallel to the line of centers with the corresponding creeping flow analytical solution [12] for the drag as a function of the particle separation distance; no such rigorous tests of hydrodynamic particle interaction appear to have been performed with other existing fluid–particle solvers. The more difficult case of hydrodynamic interaction that leads to mechanical contact is beyond the present scope of introducing the pressure boundary integral method.

2. Model formulation

Consider N_P spherical particles of radius a (Fig. 1), centered at $\mathbf{r} = \mathbf{q}_j$ ($j = 1, N_P$) inside a rectangular computational box and having translational and rotational velocities $\mathbf{U}_j(t)$ and $\mathbf{\Omega}_j(t)$. Here $\mathcal{V}(t)$ will denote the space occupied by the fluid at time t and V will denote the volume of the entire computational box. The fluid velocity $\mathbf{u} = \mathbf{u}(\mathbf{r})$ will be determined by solving the pressure-Poisson formulation of the Navier–Stokes equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{\nabla p}{\rho} + \mathbf{B} + \nu\Delta\mathbf{u}, \quad \mathbf{r}\in\mathcal{V}(t), \tag{1a}$$

$$\Delta p = -\rho\nabla\cdot(\mathbf{u}\cdot\nabla\mathbf{u}), \quad \mathbf{r}\in\mathcal{V}(t), \tag{1b}$$

where $\mathbf{B}$ is a body force, ν is the viscosity and ρ density. On the jth particle surface the no-slip boundary conditions implies:

$$\mathbf{u} = \mathbf{U}_j + a\mathbf{\Omega}_j\times\mathbf{i}_r, \quad |\mathbf{r}-\mathbf{q}_j| = a, \tag{2a}$$

where $\mathbf{i}_r \equiv (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is the local (with respect to the center of particle j) unit radial vector and (θ,ϕ) are the spherical coordinates on the particle surface (Fig. 1). Sani and Gresho [8] showed that the proper boundary condition for (1b) is the Neumann boundary condition for pressure given by the normal component of the momentum equation evaluated on the boundary. Thus, evaluating the radial component of (1a) on the particle surface and using (2a) yields the following Neumann boundary condition for pressure:

$$\frac{1}{\rho}\frac{\partial p}{\partial r} = \nu\frac{\partial^2 u_r}{\partial r^2} + \mathbf{i}_r\cdot\left(\mathbf{B} - d\mathbf{U}_j/dt\right) + a\left(\Omega_j^2 - \left(\mathbf{\Omega}_j\cdot\mathbf{i}_r\right)^2\right), \tag{2b}$$