

# A formulation for fast computations of rigid particulate flows

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## 1. Introduction

A formulation is presented for the direct numerical simulation of freely-moving rigid particles in fluids. This approach is an adaptation of the method described by Patankar *et al.* (2000), and does not rely on any model for fluid-particle interaction. The idea is to assume that the entire fluid-particle domain is a fluid and then to constrain the particle domain to move with a rigid motion. The fluid-particle motion is treated implicitly so that the mutual forces of interaction cancel because they are internal to the combined system. The formulation can be implemented by an immersed boundary and a fractional time-stepping technique. It is suitable for fast computations and can be employed for DNS, LES or RANS type simulations of turbulent particulate flows.

Numerical simulation techniques for solid-liquid flows, which do not use any model for fluid-particle interaction, have been developed over the past ten years. In these methods the fluid flow is governed by the continuity and momentum equations, whereas the particles are governed by the equation of motion for a rigid body. The flow field around each individual particle is resolved; the hydrodynamic force between the particle and the fluid is obtained from the solution and is not modeled by any drag law. These simulations, referred to as Direct Numerical Simulation (DNS) of solid-liquid flows, can be applied in numerous settings; e.g. sedimenting and fluidized suspensions, lubricated transport, hydraulic fracturing of reservoirs, slurries, understanding particle-turbulence interaction etc.

Hu *et al.* (1992), Hu (1996) and Hu *et al.* (2001) developed a finite-element method based on unstructured grids to simulate the motion of large numbers of rigid particles in two and three dimensions in Newtonian and viscoelastic fluids. This approach is based on an Arbitrary-Lagrangian-Eulerian (ALE) technique that uses a moving-mesh scheme to handle the time-dependent fluid domain. A new mesh is generated when the old one becomes too distorted, and the flow field is projected onto the new mesh. A combined fluid-particle weak formulation is used, where the hydrodynamic forces and torques on the particles are not calculated explicitly. Another numerical scheme based on the moving-mesh technique was developed by Johnson & Tezduyar (1996). They use a space-time finite-element formulation and a fully-explicit scheme in which the forces and torques on the particles are calculated explicitly to solve the equations of rigid motion.

Glowinski *et al.* (1999) presented a distributed Lagrange-multiplier/fictitious-domain method (DLM) for the direct numerical simulation of the motion of large numbers of rigid particles in Newtonian fluids. Their finite-element formulation permits the use of a fixed structured grid. This eliminates the need for remeshing the domain – a necessity in unstructured-grid-based methods. Structured grids also allow the use of fast and efficient solvers. In the DLM method the flow in the particle domain is constrained to be a rigid-

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body motion using a field of Lagrange multipliers. The constraint of rigid-body motion is represented by  $\mathbf{u} = \mathbf{U} + \boldsymbol{\Omega} \times \mathbf{r}$ , where  $\mathbf{u}$  is the velocity of the fluid at a point in the particle domain,  $\mathbf{U}$  and  $\boldsymbol{\Omega}$  are the translational and angular velocities of the particle, respectively, and  $\mathbf{r}$  is the position vector of the point with respect to the particle centroid. The fluid-particle motion is treated implicitly using a combined weak formulation in which the mutual forces cancel.

A new DLM formulation for particulate flows was later presented by Patankar *et al.* (2000). In their approach, the rigid motion is imposed by constraining the deformation-rate tensor within the particle domain to be zero. This eliminates  $\mathbf{U}$  and  $\boldsymbol{\Omega}$  as variables from the coupled system of equations. This formulation recognizes that the rigidity constraint results in a stress field inside a rigid solid just as there is pressure in an incompressible fluid. The DLM formulations of Glowinski *et al.* (1999) and Patankar *et al.* (2000) were implemented by using a Marchuk-Yanenko fractional-step scheme for time discretization. A finite-element method was used.

The lattice-Boltzmann method (LBM) is an alternative scheme for simulating fluid flow problems. In LBM, simplified kinetic models, which incorporate the essential physics of the microscopic and mesoscopic equations, are constructed. The LBM has been adapted to simulate the motion of solid particles in Newtonian fluids: see Ladd (1994a), Ladd (1994b). Another approach, which uses an analytic solution near the particle and a numerical procedure away from it, was developed by Takagi *et al.* (2001).

Pan & Banerjee (1997) performed DNS of fluid-particle motion in turbulent flows. They solved the Navier-Stokes equations with an external body-source term that models the no-slip boundary condition on the surface of the particles. The source term is imposed only in the particle domain. The particle size is comparable to the computational mesh size. They use a pseudo-spectral method to solve the governing equations. All the calculations are carried out in the wave space, except for the evaluation of the non-linear advection term and the external body-source term which imposes the no-slip condition on the particle surfaces. While these results were helpful in the investigation of particle-turbulence interaction, the formulation of the problem was *ad hoc*. The expression for the source term in the particle domain was not based on rigorous theory. Iterations were required to arrive at a correct source term at each time step. Only the particle translational motion was considered, and a rigorous formulation should include the particle rotation.

Kajishima *et al.* (1999) developed an immersed-boundary approach for the DNS of turbulent rigid particulate flows. They added a source term in the fluid equation to account for the no-slip boundary condition on the fluid-particle interface. The fluid-particle momentum coupling was explicit, i.e. the fluid equations were solved with the latest known velocities of the particles and then the particle equations were solved with the latest known velocity field of the fluid. This procedure is often undesirable as it is unstable under certain circumstances: see Hu *et al.* (1992). The fully-explicit momentum coupling scheme of Kajishima *et al.* (1999) is first-order accurate in time. These issues can be particularly important in the development of robust and accurate schemes for the DNS of turbulent particulate flows.

The ALE and DLM formulations have been implemented for laminar flow conditions. Although the DLM approach has been successfully used for computations with up to 1204 spheres in three dimensions – see Pan *et al.* (2001) – the implicit coupling of fluid-particle momentum equations slows down the solution procedure. This is critical for DNS of turbulent particulate flows or for performing simulations with thousands of particles.

Methods based on explicit coupling can be unstable. In this paper we develop a technique for efficient computations of high and low Reynolds number particulate flows. The new formulation allows fast computations of particulate flows, and at the same time has implicit coupling of fluid-particle momentum equations. It can be easily implemented by using finite-element, finite-difference or finite-volume methods. It is suitable for DNS, LES or RANS type simulations of turbulent particulate flows.

In Section 2, the numerical scheme will be presented. Results will be presented in Section 3.

## 2. The numerical scheme

The approach in this paper is an adaptation of the formulation of Patankar *et al.* (2000). In this Section, we will first present their formulation and then introduce our new approach as a modification of their method.

### 2.1. The stress-DLM formulation of Patankar *et al.* (2000)

Let  $V$  be the computational space, which includes both the fluid and the particle domains. Let  $P(t)$  be the particle domain. Let the fluid boundary, not shared with the particle, be denoted by  $\partial V$ . For simplicity we assume that a Dirichlet boundary condition is imposed on  $\partial V$ . The equations are presented by assuming only one particle in the computational domain. The formulation can be easily generalized beyond these assumptions. The body force is assumed to be constant so that there is no net torque acting on the particle. The governing equations for fluid motion are given by:

$$\rho_f \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot \boldsymbol{\Sigma} + \rho_f \mathbf{g} \quad \text{in } V \setminus \overline{P(t)}, \quad (2.1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } V \setminus \overline{P(t)}, \quad (2.2)$$

$$\mathbf{u} = \mathbf{u}_{\partial V}(t) \quad \text{on } \partial V, \quad (2.3)$$

$$\mathbf{u} = \mathbf{u}_i \quad \& \quad \boldsymbol{\Sigma} \cdot \mathbf{n} = \mathbf{t} \quad \text{on } \partial P(t), \quad (2.4)$$

$$\mathbf{u}|_{t=0} = \mathbf{u}_0(\mathbf{x}) \quad \text{in } V \setminus \overline{P(0)}, \quad (2.5)$$

where  $\rho_f$  is the fluid density,  $\mathbf{u}$  is the fluid velocity,  $\mathbf{g}$  is the acceleration due to gravity,  $\mathbf{n}$  is the unit outward normal on the particle surface,  $\mathbf{u}_i$  is the velocity at the fluid-particle interface  $\partial P(t)$  and  $\boldsymbol{\Sigma}$  is the stress tensor. The initial velocity  $\mathbf{u}_0$  should satisfy Eq. (2.2). The boundary velocity in Eq. (2.3) should satisfy the compatibility condition due to Eq. (2.2). For an incompressible fluid the divergence-free constraint Eq. (2.2) gives rise to pressure in the fluid. The stress tensor is given by:

$$\boldsymbol{\Sigma} = -p\mathbf{I} + \boldsymbol{\Pi} \quad (2.6)$$

where  $\mathbf{I}$  is the identity tensor,  $p$  is the pressure and  $\boldsymbol{\Pi}$  is the extra stress tensor. For a Newtonian fluid  $\boldsymbol{\Pi}$  represents the viscous stress, whereas for a viscoelastic fluid it represents the viscous and elastic stresses in the fluid. The extra stress depends on the deformation rate of the fluid at a given location. In a viscoelastic fluid it also depends on the history of deformation.

Patankar *et al.* (2000) treated the particle as a fluid with an additional constraint to impose the rigid motion. The governing equations for particle motion are:

$$\rho_s \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot \boldsymbol{\Sigma} + \rho_s \mathbf{g} \quad \text{in } P(t), \quad (2.7)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } P(t), \quad (2.8)$$

$$\nabla \cdot (\mathbf{D}[\mathbf{u}]) = \mathbf{0} \quad \text{in } P(t) \quad \& \quad \mathbf{D}[\mathbf{u}] \cdot \mathbf{n} = \mathbf{0} \quad \text{on } \partial P(t), \quad (2.9)$$

$$\mathbf{u} = \mathbf{u}_i \quad \& \quad \boldsymbol{\Sigma} \cdot \mathbf{n} = \mathbf{t} \quad \text{on } \partial P(t), \quad (2.10)$$

$$\mathbf{u}|_{t=0} = \mathbf{u}_0(\mathbf{x}) \quad \text{in } P(0), \quad (2.11)$$

where  $\rho_s$  is the particle density. Equation (2.9) represents the rigidity constraint that sets the deformation-rate tensor,  $\mathbf{D}[\mathbf{u}] = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ , in the particle domain equal to zero. The initial velocity  $\mathbf{u}_0$  should satisfy Eq. (2.9). The rigidity constraint ensures that the velocity field is divergence-free. Hence Eq. (2.8) is a redundant constraint. Nevertheless, it is retained in order to facilitate the application of the fluid equations in the entire domain. The stress inside the particle – see Patankar *et al.* (2000) – is given by

$$\boldsymbol{\Sigma} = -p\mathbf{I} + \mathbf{D}[\boldsymbol{\Lambda}] + \boldsymbol{\Pi} \quad (2.12)$$

where  $\boldsymbol{\Lambda}$  is the Lagrange multiplier due to the rigidity constraint and  $\boldsymbol{\Pi}$  is the extra stress tensor which depends on the deformation rate. The extra stress is zero inside the particle domain since the deformation rate is constrained to be zero.

A two-dimensional case is considered for simplicity. The combined weak form of the fluid-particle equations is given by:

For  $t > 0$ , find  $\mathbf{u} \in W_u$ ,  $p \in L_0^2(V)$ ,  $\boldsymbol{\Lambda} \in H^1(P(t))^2$  satisfying

$$\begin{aligned} & \int_V \rho_f \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x} - \int_V p (\nabla \cdot \mathbf{v}) \, d\mathbf{x} + \int_V q (\nabla \cdot \mathbf{u}) \, d\mathbf{x} \\ & + \int_V \boldsymbol{\Pi} : \mathbf{D}[\mathbf{v}] \, d\mathbf{x} + \int_{P(t)} (\rho_s - \rho_f) \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x} \\ & + \int_{P(t)} \mathbf{D}[\boldsymbol{\Lambda}] : \mathbf{D}[\mathbf{v}] \, d\mathbf{x} + \int_{P(t)} \mathbf{D}[\boldsymbol{\Psi}] : \mathbf{D}[\mathbf{u}] \, d\mathbf{x} = 0, \\ & \forall \mathbf{v} \in W_0, \quad q \in L_0^2(V) \quad \& \quad \boldsymbol{\Psi} \in H^1(P(t))^2, \end{aligned} \quad (2.13)$$

where

$$W_u(t) = \{\mathbf{v} | \mathbf{v} \in H^1(V)^2, \mathbf{v} = \mathbf{u}_{\partial V}(t) \quad \text{on } \partial V\},$$

$$W_0(t) = \{\mathbf{v} | \mathbf{v} \in H^1(V)^2, \mathbf{v} = \mathbf{0} \quad \text{on } \partial V\},$$

$$L_0^2(V) = \{q \in L^2(V) | \int_V q \, d\mathbf{x} = 0\},$$

and  $\mathbf{v}$ ,  $\boldsymbol{\Psi}$  &  $q$  are the variations of  $\mathbf{u}$ ,  $\boldsymbol{\Lambda}$  &  $p$ , respectively. The initial conditions are given by Eq. (2.5) and Eq. (2.11). The fluid-particle interface condition is internal to the combined system. Hence there are no explicit interface-force or velocity terms in Eq. (2.13). The particle translational and angular velocities are not present in the combined form Eq. (2.13). This is especially convenient in a three-dimensional case with irregularly-shaped bodies, for which there is added complexity due to the nonlinear nature of the angular-momentum equation. Equation (2.13) is solved by a Marchuk-Yanenko fractional-step scheme. The algorithm based on this scheme, given by Patankar *et al.* (2000), is:

(1) Calculate particle velocity: given  $\mathbf{u}^n$  and  $P(t_n)$ , find the translational velocity,  $\mathbf{U}^n$ , of the particle:

$$M\mathbf{U}^n = \int_{P(t^n)} \rho_s \mathbf{u}^n \, d\mathbf{x}, \quad (2.14)$$

where  $M$  is the mass of the particle. For a non-circular particle it is necessary to update the angular position of the particle. The angular velocity,  $\boldsymbol{\Omega}^n$ , of the particle is given by

$$\mathbf{I}_p \boldsymbol{\Omega}^n = \int_{P(t^n)} \mathbf{r} \times \rho_s \mathbf{u}^n d\mathbf{x}, \quad (2.15)$$

where  $\mathbf{I}_p$  is the moment of inertia of the particle.

(2) Explicit update of particle position: Compute  $\mathbf{X}^{n+1}$  by the following procedure:

Set  $\mathbf{X}^{n+1,0} = \mathbf{X}^n$ .

do  $k = 1, K$

$$\mathbf{X}^{*n+1,k} = \mathbf{X}^{n+1,k-1} + \left( \frac{\mathbf{U}^n + \mathbf{U}^{n-1}}{2} \right) \left( \frac{\Delta t}{K} \right) \quad (2.16)$$

$$\mathbf{X}^{n+1,k} = \mathbf{X}^{*n+1,k} + \left( \frac{\mathbf{F}(\mathbf{X}^{n+1,k-1}) + \mathbf{F}(\mathbf{X}^{*n+1,k})}{2M} \right) \left( \frac{\Delta t^2}{2K^2} \right) \quad (2.17)$$

enddo

Set  $\mathbf{X}^{n+1} = \mathbf{X}^{n+1,K}$ , this also gives  $P(t^{n+1})$ .

Set

$$\mathbf{A}_c^{n+1} = \frac{2}{\Delta t^2} (\mathbf{X}^{n+1} - \mathbf{X}^n - \left( \frac{\mathbf{U}^n + \mathbf{U}^{n-1}}{2} \right) \Delta t), \quad (2.18)$$

where  $\mathbf{X}$  is the position of the particle centroid and  $\mathbf{F}$  denotes the collision force acting on the particles to prevent them from penetrating each other or the walls of the domain.  $\mathbf{A}_c$  is the acceleration of the particle due to collision. This term provides an additional body force acting on the particle and is included in the combined momentum equation to be solved in the subsequent steps. Details of the collision-force model used in this paper can be found in Glowinski *et al.* (1999). An additional equation to update the angular position is required for non-circular particles.

(3) Fractional step 1: Find  $\mathbf{u}^{n+1/3} \in W_u(t^{n+1})$  and  $p^{n+1/3} \in L_0^2(V)$  satisfying

$$\begin{aligned} & \int_V \rho_f \left( \frac{\mathbf{u}^{n+1/3} - \mathbf{u}^n}{\Delta t} - \mathbf{g} \right) \cdot \mathbf{v} d\mathbf{x} - \int_V p^{n+1/3} (\nabla \cdot \mathbf{v}) d\mathbf{x} + \int_V q (\nabla \cdot \mathbf{u}^{n+1/3}) d\mathbf{x} \\ & + \alpha \int_V 2\eta \mathbf{D}[\mathbf{u}^{n+1/3}] : \mathbf{D}[\mathbf{v}] d\mathbf{x} = 0, \quad \forall \mathbf{v} \in W_0 \quad \& \quad q \in L_0^2(V). \end{aligned} \quad (2.19)$$

(4) Fractional step 2: Find  $\mathbf{u}^{n+2/3} \in W_u(t^{n+1})$  satisfying

$$\begin{aligned} & \int_V \rho_f \left( \frac{\mathbf{u}^{n+2/3} - \mathbf{u}^{n+1/3}}{\Delta t} + (\mathbf{u}^{n+2/3} \cdot \nabla) \mathbf{u}^{n+2/3} \right) \cdot \mathbf{v} d\mathbf{x} \\ & + \beta \int_V 2\eta \mathbf{D}[\mathbf{u}^{n+2/3}] : \mathbf{D}[\mathbf{v}] d\mathbf{x} = 0, \quad \forall \mathbf{v} \in W_0. \end{aligned} \quad (2.20)$$

(5) Fractional step 3: Find  $\mathbf{u}^{n+1} \in W_u(t^{n+1})$  and  $\boldsymbol{\Lambda}^{n+1} \in H^1(P(t^{n+1}))^2$  satisfying

$$\begin{aligned} & \int_V \rho_f \left( \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+2/3}}{\Delta t} \right) \cdot \mathbf{v} d\mathbf{x} + \gamma \int_V 2\eta \mathbf{D}[\mathbf{u}^{n+1}] : \mathbf{D}[\mathbf{v}] d\mathbf{x} - \int_{P(t^{n+1})} \rho_s \mathbf{A}_c^{n+1} \cdot d\mathbf{x} \\ & + \int_{P(t^{n+1})} \mathbf{D}[\boldsymbol{\Lambda}^{n+1}] : \mathbf{D}[\mathbf{v}] d\mathbf{x} + \int_{P(t^{n+1})} \mathbf{D}[\boldsymbol{\Psi}] : \mathbf{D}[\mathbf{u}^{n+1}] d\mathbf{x} \\ & + \int_{P(t^{n+1})} (\rho_s - \rho_f) \left( \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^{n+2/3} \cdot \nabla) \mathbf{u}^{n+2/3} - \mathbf{g} \right) \cdot \mathbf{v} d\mathbf{x} = 0, \end{aligned}$$

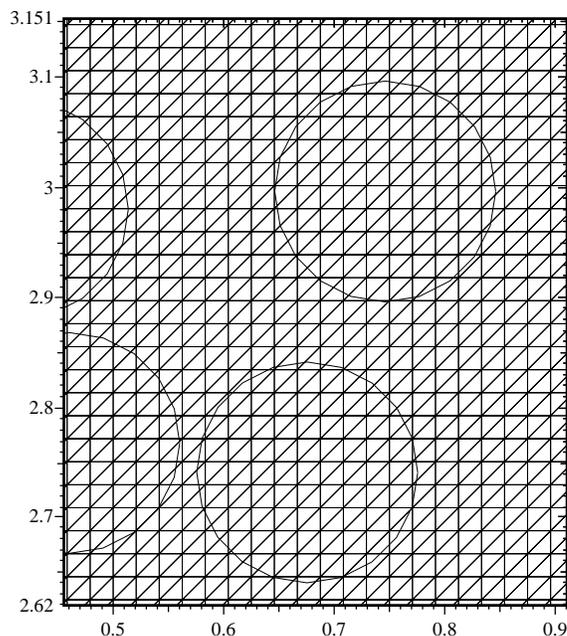


FIGURE 1. A fixed uniform triangular mesh spanning the fluid-particle domain. The circles indicate particle domains.  $\Lambda$  is defined on a triangular mesh (not shown in the figure) moving with the particles.

$$\forall \mathbf{v} \in W_0, \quad \Psi \in H^1(P(t^{n+1}))^2. \quad (2.21)$$

$\Pi$  is replaced by the Newtonian stress with constant viscosity and is split into the three fractional steps such that  $\alpha + \beta + \gamma = 1$ . Patankar *et al.* (2000) and Glowinski *et al.* (1999) performed simulations with  $\gamma = 0$ . A fixed uniform triangular mesh was used to solve Eq. (2.19) & Eq. (2.20) over the entire domain (e.g. Fig. 1). To solve Eq. (2.21),  $\Lambda$  was defined on a triangular mesh moving with the particles. A linear interpolation was used to project  $\Lambda$  from the particle mesh to the uniform background mesh and to project  $\mathbf{u}$  from the background mesh to the particle mesh. The above is a first-order time-discretization scheme. The first fractional step, Eq. (2.19), is the classical Stokes-like problem and is solved using a conjugate-gradient method. The second fractional step, Eq. (2.20), defines a nonlinear problem for velocity which is solved by using a least-squares conjugate-gradient algorithm. The third fractional step, Eq. (2.21), is solved by a Uzawa conjugate-gradient algorithm. Details are given in Patankar *et al.* (2000) and Glowinski *et al.* (1999). A Galerkin finite-element method was used.

## 2.2. A new approach to impose the rigidity constraint

The last fractional step, Eq. (2.21), adds computational cost to the solution procedure. This is the additional computational time spent to account for the presence of the particles. The last step is a projection of the velocity field on to a rigid motion in the particle domain. When  $\gamma = 0$ , the velocity is corrected only in the particle domains. This introduces an error in the form of small slip at the fluid-particle interface. Smaller time steps are preferable to reduce this error, especially when the particle and fluid densities are not matched. One way to minimize it is to add the buoyant-weight term in the first

or second fractional step. In the numerical method the slip is smeared on the length scale of the smallest grid size. Indeed, if  $\gamma \neq 0$  then there is no slip on the interface but it increases the computational cost. A Uzawa conjugate gradient algorithm is used in the current implementations of the DLM formulation: see Glowinski *et al.* (1999) and Patankar *et al.* (2000). The correct velocity field and the corresponding Lagrange multiplier field are obtained simultaneously through an iterative procedure. Here we present a fast projection scheme that eliminates the need to solve the last fractional step by an iterative procedure when  $\gamma = 0$ . Even when  $\gamma \neq 0$ , the scheme presented can provide a significant reduction in the computational cost, at each iteration, as compared to the current implementations.

The last fractional step Eq. (2.21), with  $\gamma = 0$ , can be rewritten as

$$\int_{P(t^{n+1})} \rho_s \left( \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+2/3}}{\Delta t} \right) \cdot \mathbf{v} \, d\mathbf{x} = \int_{P(t^{n+1})} \mathbf{S} \cdot \mathbf{v} \, d\mathbf{x} + \int_{P(t^{n+1})} \mathbf{f} \cdot \mathbf{v} \, d\mathbf{x}, \quad (2.22)$$

where

$$\begin{aligned} \int_{P(t^{n+1})} \mathbf{S} \cdot \mathbf{v} \, d\mathbf{x} &= \int_{P(t^{n+1})} \rho_s \mathbf{A}_c^{n+1} \cdot d\mathbf{x} \\ &- \int_{P(t^{n+1})} (\rho_s - \rho_f) \left( \frac{\mathbf{u}^{n+2/3} - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^{n+2/3} \cdot \nabla) \mathbf{u}^{n+2/3} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x}, \\ &\& \\ \int_{P(t^{n+1})} \mathbf{f} \cdot \mathbf{v} \, d\mathbf{x} &= - \int_{P(t^{n+1})} \mathbf{D}[\mathbf{\Lambda}^{n+1}] : \mathbf{D}[\mathbf{v}] \, d\mathbf{x} \\ &= \int_{P(t^{n+1})} (\nabla \cdot \mathbf{D}[\mathbf{\Lambda}^{n+1}]) \cdot \mathbf{v} \, d\mathbf{x} - \int_{\partial P(t^{n+1})} (\mathbf{D}[\mathbf{\Lambda}^{n+1}] \cdot \mathbf{n}) \cdot \mathbf{v} \, d\mathbf{A}. \end{aligned}$$

$\mathbf{S}$  is a source term that can be calculated explicitly, based on known values of the variables, and  $\mathbf{f}$  is a source term, to be determined, due to the rigidity constraint. The weak form of the rigidity constraint Eq. (2.9) should be solved simultaneously with Eq. (2.22). Let us consider the strong form of Eq. (2.22), applicable in the particle domain:

$$\rho_s \left( \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+2/3}}{\Delta t} \right) = \mathbf{S} + \mathbf{f}. \quad (2.23)$$

The solution of Eq. (2.23) can be obtained in two steps:

(a) Find  $\hat{\mathbf{u}}$  by solving

$$\rho_s \left( \frac{\hat{\mathbf{u}} - \mathbf{u}^{n+2/3}}{\Delta t} \right) = \mathbf{S}. \quad (2.24)$$

(b) Find  $\mathbf{u}^{n+1}$  by projecting  $\hat{\mathbf{u}}$  on to a rigid body motion

$$\rho_s \left( \frac{\mathbf{u}^{n+1} - \hat{\mathbf{u}}}{\Delta t} \right) = \mathbf{f}. \quad (2.25)$$

$\hat{\mathbf{u}}$  is an intermediate velocity field in the particle domain. Solution of Eq. (2.24) is straightforward. To solve for  $\mathbf{u}^{n+1}$  we need  $\mathbf{f}$ . An equation for  $\mathbf{f}$  can be obtained by using Eq. (2.9). We get

$$\begin{aligned} \nabla \cdot (\mathbf{D}[\mathbf{u}^{n+1}]) &= \nabla \cdot \left( \mathbf{D} \left[ \hat{\mathbf{u}} + \frac{\mathbf{f} \Delta t}{\rho_s} \right] \right) = \mathbf{0}, \\ \& \quad \mathbf{D}[\mathbf{u}^{n+1}] \cdot \mathbf{n} &= \mathbf{D} \left[ \hat{\mathbf{u}} + \frac{\mathbf{f} \Delta t}{\rho_s} \right] \cdot \mathbf{n} = \mathbf{0}. \end{aligned} \quad (2.26)$$

The above equation implies that  $\hat{\mathbf{u}} + (\mathbf{f}\Delta t)/\rho_s$  is a rigid-body motion, but it gives no information about what this rigid motion should be. In fact, this rigid motion is the solution that we are seeking because  $\hat{\mathbf{u}} + (\mathbf{f}\Delta t)/\rho_s = \mathbf{u}^{n+1}$ .

We can obtain the rigid motion by imposing an additional condition that, in the projection step Eq. (2.25), the total linear and angular momenta in the individual particle domains should be conserved. The required solution is then obtained by the following procedure:

(i) Split  $\hat{\mathbf{u}}$  as:  $\hat{\mathbf{u}} = \hat{\mathbf{u}}_R + \hat{\mathbf{u}}'$ , where  $\hat{\mathbf{u}}_R$  is the velocity field of a rigid motion. It is given by:

$$\begin{aligned}\hat{\mathbf{u}}_R &= \hat{\mathbf{U}} + \hat{\mathbf{\Omega}} \times \mathbf{r}, \\ M\hat{\mathbf{U}} &= \int_P \rho_s \hat{\mathbf{u}} d\mathbf{x} \quad \& \quad \mathbf{I}_p \hat{\mathbf{\Omega}} = \int_P \mathbf{r} \times \rho_s \hat{\mathbf{u}} d\mathbf{x},\end{aligned}\quad (2.27)$$

where  $\mathbf{r}$  is the position vector of a point with respect to the centroid of the particle. This computational step is cheap since it is merely an addition (integration).

(ii) Since the linear and angular momenta should be conserved in the projection step, set  $\mathbf{u}^{n+1} = \hat{\mathbf{u}}_R$  in the particle domain. This is the required solution. Note that  $\mathbf{f} = -(\rho_s \hat{\mathbf{u}}')/\Delta t$ .

The solution procedure above requires no iterations and is computationally cheap. We replace the last fractional step Eq. (2.21) in our previous work by this equivalent procedure. The results are presented in Section 3.

### 2.3. Application to turbulent particulate flows

The new formulation presented above is suitable for finite-volume or finite-difference immersed-boundary techniques for the simulation of freely-moving particles. The key issue that we address in this formulation is the fast implementation of the rigidity constraint, irrespective of the type of equations used to describe the fluid. Hence, it can be used in a DNS, LES or RANS type approach. As an example, we present a fractional step scheme similar to the approach of Kajishima *et al.* (1999) who performed DNS of turbulent flows with rigid particles.

For simplicity, we assume  $\rho_s = \rho_f = \rho$  and a Newtonian fluid with constant viscosity. The scheme can be generalized to the unmatched-density case as in Section 2.2 above. The momentum equation is

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \eta \nabla^2 \mathbf{u} + \rho \mathbf{g} + \mathbf{f}, \quad (2.28)$$

where  $\mathbf{f}$  is the additional source term due to the rigidity constraint Eq. (2.9) in the particle domain. In the formulation of Patankar *et al.* (2000) the source term is  $\mathbf{f} = \nabla \cdot (\mathbf{D}[\mathbf{\Lambda}])$ . The velocity field should be divergence-free in the entire domain. The above equations are to be solved on a fixed grid spanning the entire fluid/particle domain. A fractional-step scheme is summarized below:

(1) Find  $\bar{\mathbf{u}}$  by solving the following equation over the entire domain

$$\rho \left( \frac{\bar{\mathbf{u}} - \mathbf{u}^n}{\Delta t} \right) = \frac{1}{2} (3\mathbf{H}^n - \mathbf{H}^{n-1}) - \nabla p^n + \frac{1}{2} \eta \nabla^2 (\bar{\mathbf{u}} + \mathbf{u}^n) + \rho \mathbf{g}, \quad (2.29)$$

where

$$\mathbf{H} = -\rho (\mathbf{u} \cdot \nabla) \mathbf{u}.$$

The Adams-Bashforth method is used for the convection term and the Crank-Nicolson scheme is used for the viscous term.

(2) The projection of  $\bar{\mathbf{u}}$  on to a divergence-free velocity field  $\tilde{\mathbf{u}}$  (applicable in the entire domain):

$$\nabla^2 G = \frac{\rho \nabla \cdot \bar{\mathbf{u}}}{\Delta t}, \quad (2.30)$$

$$\rho \left( \frac{\tilde{\mathbf{u}} - \bar{\mathbf{u}}}{\Delta t} \right) = -\nabla G. \quad (2.31)$$

(3) The projection of  $\tilde{\mathbf{u}}$  on to a rigid motion in the particle domain:

$$\begin{aligned} \text{Split } \tilde{\mathbf{u}} &= \tilde{\mathbf{u}}_R + \tilde{\mathbf{u}}', \quad \text{where } \tilde{\mathbf{u}}_R = \tilde{\mathbf{U}} + \tilde{\mathbf{\Omega}} \times \mathbf{r}, \\ M\tilde{\mathbf{U}} &= \int_P \rho_s \tilde{\mathbf{u}} d\mathbf{x} \quad \& \quad \mathbf{I}_p \tilde{\mathbf{\Omega}} = \int_P \mathbf{r} \times \rho_s \tilde{\mathbf{u}} d\mathbf{x}, \end{aligned} \quad (2.32)$$

$$\mathbf{f} = \frac{\phi \rho (\tilde{\mathbf{u}}_R - \tilde{\mathbf{u}})}{\Delta t}, \quad (2.33)$$

$$\rho \left( \frac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}}{\Delta t} \right) = \mathbf{f}, \quad (2.34)$$

where  $\phi$  is the particle volume fraction in a control volume associated with a given grid point: see Kajishima *et al.* (1999). Equations (2.32)-(2.34) are based on the new projection scheme presented in Section 2.2. As in the approach of Kajishima *et al.* (1999), we calculate  $\mathbf{f}$  on the fixed grid nodes.

The advantage of our method is that the fluid and particle velocities are solved simultaneously, unlike the technique of Kajishima *et al.* (1999) where the fluid-particle momentum coupling was explicit. Explicit coupling is often undesirable since it can lead to instabilities: see e.g. Hu *et al.* (1992). The additional computational cost in step 3 will be negligible compared to the time required to solve the fluid equations over the entire domain.

A grid over the particle domain is not essential in the above approach. Integrations are required over the particle domains (Eq. 2.32) which do not conform with the fixed grid. The accuracy of the solution in the vicinity of the particle boundary depends on the interpolation schemes used in these integrations. The order of accuracy and the interpolation scheme can be improved, and need further investigation. Nevertheless, we believe that this is a promising approach for the simulation of large numbers of moving particles and for turbulent particulate flows, especially in light of the simulations of Kajishima *et al.* (1999).

### 3. Results

We validate our new formulation by presenting preliminary results of the sedimentation of two circular particles in a Newtonian fluid. We use the numerical scheme of Patankar *et al.* (2000), the only difference being that the new rigid-motion-projection scheme, in Section 2.2, is used instead of Eq. (2.21). A finite-element method is used with a triangular grid (Fig. 1).

It is known that two particles dropped close to each other in a Newtonian fluid undergo drafting, kissing and tumbling; see Fortes *et al.* (1987). This simulation has been used as a test case in our previous work.

We consider a channel 2 cm wide ( $x$ -direction) and 8 cm tall ( $y$ -direction). The fluid viscosity is 0.01 g/cm-s and the density is 1 g/cc. The particle density is 1.01 g/cc and the particle radius is 0.1 cm. Gravity acts in the negative  $y$ -direction. The simulation is

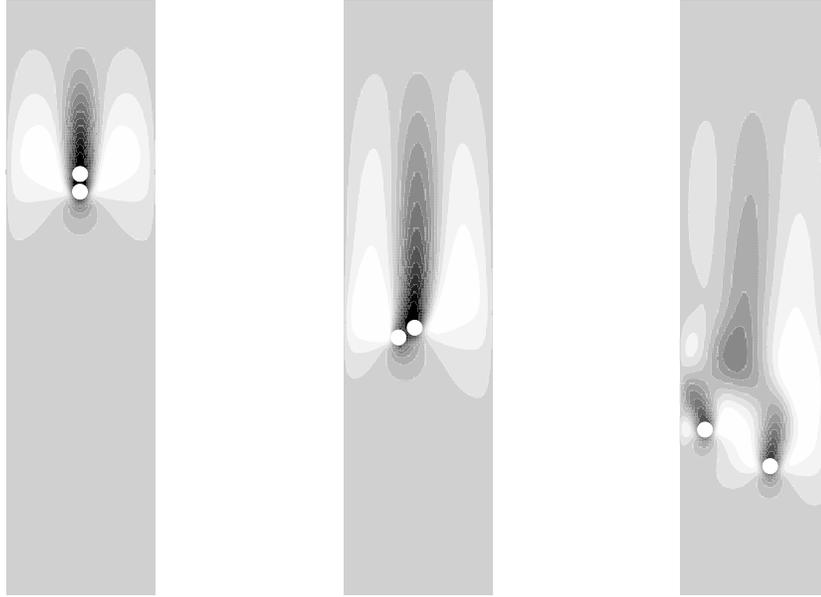


FIGURE 2. Numerical simulation of drafting, kissing and tumbling of particles in a Newtonian fluid. Contour plots of the vertical velocity in the fluid domain are shown at times  $t = 1.5s$ ,  $2s$  &  $5s$ , respectively. Darker shades imply higher downward velocity of the fluid. The particles are shown by white circles to make them visible; white color in the particle domains do not represent the vertical velocity.

started at  $t = 0$  s by dropping two particles at the center of the channel at a height of 7.2 cm and 6.8 cm, respectively. The fixed (background) mesh size for velocity is 1/96 cm and for pressure is 1/48 cm (a coarser mesh is used for pressure to satisfy the Babuska-Brezzi condition). The particle mesh size is 1/96 cm. The time step is 0.0025 s.

Figure 2 shows the numerical simulation of drafting, kissing and tumbling of particles in a Newtonian fluid; in agreement with experimental observations. Figure 3 shows the plot of particle velocities in the vertical ( $y$ -) direction. As expected the lagging particle moves with a higher velocity and catches up with the particle in the front (drafting). The particles fall one behind the other with almost the same velocity for some time. This configuration is unstable in a Newtonian fluid. The particles eventually tumble and move apart. Convergence tests were done by changing the time step and the mesh resolution; similar results were obtained.

The numerical results are compared with those obtained using the original formulation of Patankar *et al.* (2000). The vertical-velocity plot of Patankar *et al.* (2000) differs quantitatively from Fig. 3 shown here, after the kissing and tumbling phases begin. In their case, tumbling is initiated earlier thus giving a different graph. This is inherent in these simulations, since the tumbling process is a realization of an instability and can be affected by the accuracy of the solution procedure and the modeling of the collision

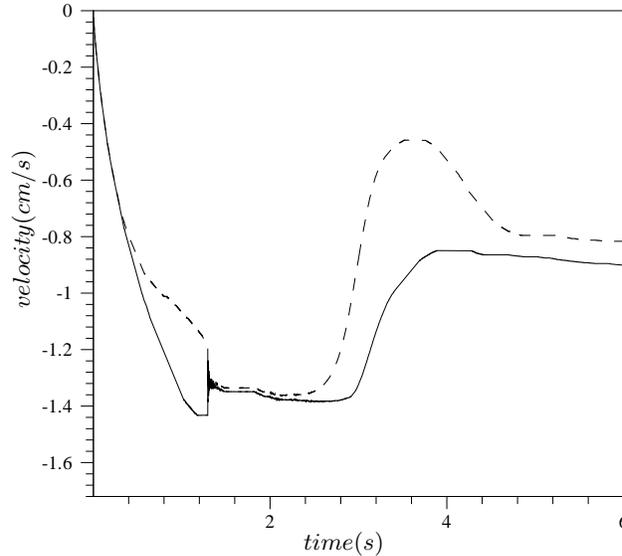


FIGURE 3. Vertical velocity of the particles. The solid line represents the velocity of the leading particle and the dashed line represents the velocity of the lagging particle.

force: see Singh, Joseph & Hesla (2001). Similar differences were also observed by T.-W. Pan (private communication).

#### 4. Conclusions

We have developed a fast projection scheme to impose the rigidity constraint for the direct numerical simulation of rigid particulate flows. The new formulation is suitable for finite-volume or finite-difference immersed boundary techniques. The scheme is implemented by modifying the approach of Patankar *et al.* (2000). Numerical simulation of drafting, kissing and tumbling of particles has been done to validate the method.

This method can form a basis for fast computations of large numbers of moving particles. Such simulations can be used to develop models of solid-liquid flows. The new approach is also suitable for the direct numerical simulation of turbulent particulate flows since it directly improves upon the previous efforts of Kajishima *et al.* (1999). The technique is not restricted to any constitutive model for the suspending fluid. Hence, it can also be used in LES or RANS type simulations.

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## REFERENCES

- FORTES, A., JOSEPH, D. D. & LUNDGREN, T. S. 1987 Nonlinear mechanics of fluidization of beds of spherical particles. *J. Fluid Mech.* **177**, 467-483.
- GLOWINSKI, R., PAN, T.-W., HESLA, T. I. & JOSEPH, D. D. 1999 A distributed Lagrange multiplier/fictitious domain method for particulate flows. *Int. J. Multiphase Flow* **25**, 755-794.
- HU, H. H. 1996 Direct simulation of flows of solid-liquid mixtures. *Int. J. Multiphase Flow* **22**, 335-352.
- HU, H. H., JOSEPH, D. D. & CROCHET, M. J. 1992 Direct numerical simulation of fluid particle motions. *Theor. Comp. Fluid Dyn.* **3**, 285-306.
- HU, H. H., PATANKAR, N. A. & ZHU, M. Y. 2001 Direct numerical simulations of fluid-solid systems using Arbitrary Lagrangian-Eulerian technique. *J. Comput. Phys.* **169**, 427-462.
- JOHNSON, A. & TEZDUYAR, T. E. 1996 Simulation of multiple spheres falling in a liquid-filled tube. *Comp. Meth. Appl. Mech. Eng.* **134**, 351-373.
- KAJISHIMA, T., TAKIGUCHI, S. & MIYAKE, Y. 1999 Modulation and subgrid scale modeling of gas-particle turbulent flow. *Recent Advances in DNS & LES*, (D. Knight & L. Sakell, eds.), Kluwer Academic, 235-244.
- LADD, A. J. C. 1994a Numerical simulation of particulate suspensions via a discretized Boltzmann equation. I. Theoretical foundation. *J. Fluid Mech.* **271**, 285-309.
- LADD, A. J. C. 1994b Numerical simulation of particulate suspensions via a discretized Boltzmann equation. I. Numerical results. *J. Fluid Mech.* **271**, 311-339.
- PAN, T.-W., JOSEPH, D. D., BAI, R., GLOWINSKI, R. & SARIN, V. 2001 Fluidization of 1204 spheres: simulation and experiment. *J. Fluid Mech.* to appear.
- PAN, Y. & BANERJEE, S. 1997 Numerical investigation of the effects of large particles in wall turbulence. *Phys. Fluids* **9**, 3786-3807.
- PATANKAR, N. A., SINGH, P., JOSEPH, D. D., GLOWINSKI, R. & PAN, T.-W. 2000 A new formulation of the distributed Lagrange multiplier/fictitious domain method for particulate flows. *Int. J. Multiphase Flow* **26**, 1509-1524.
- SINGH, P., HESLA, T. I. & JOSEPH, D. D. 2001 Modified distributed Lagrange multiplier/fictitious domain method for particulate flows with collisions. *Int. J. Multiphase Flow*, in press.
- TAKAGI, S., OǒUZ, H. N., ZHANG, Z. & PROSPERETTI, A. 2001 PHYSALIS: A new method for particle simulation. Part II: Two-dimensional Navier-Stokes flow around cylinders. *J. Comput. Phys.*, submitted.