Distributed Lagrange Multiplier Methods for Particulate Flows

R. Glowinski[1], T. Hesla[2], D. D. Joseph[2], T.-W. Pan[3], and J. Périaux[4]

[1]*Department of Mathematics, University of Houston, Houston, Texas 77204 USA, and Université P. et M. Curie, Paris, France.*
[2]*Department of Aerospace and Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, USA.*
[3]*Department of Mathematics, University of Houston, Houston, Texas 77204, USA.*
[4]*Dassault Aviation, 92214 Saint-Cloud, France.*

Abstract

In this article we discuss the application of a Lagrange multiplier based fictitious domain method to the numerical simulation of incompressible viscous flow modelled by the Navier-Stokes equations around moving bodies. The solution method combines finite element approximations, time discretization by operator splitting and conjugate gradient algorithms for the solution of the linearly constrained quadratic minimization problems coming from the splitting method. The results of numerical experiments for two sedimenting cylinders in a two-dimensional channel are presented.

1. INTRODUCTION

Fictitious domain methods is a general term which covers in fact a large variety of solution methods for Partial Differential Equations; one of those fictitious domain methods uses *Lagrange multipliers* and regular structured meshes (which are not boundary fitted) over a simple shape auxiliary domain (the fictitious domain) to enforce *Dirichlet boundary conditions.* Glowinski, Pan and Périaux (1994 & 1995) have used finite element methods combined with Lagrange multiplier based fictitious domain techniques to compute the solution of elliptic problems with Dirichlet boundary conditions and applied these methods for solving some nonlinear time dependent problems, namely the flow of a viscous-plastic medium in a cylindrical pipe, Ginzburg-Landau equations, and external incompressible viscous flow modelled by the Navier-Stokes equations. For the simulation of flows around moving rigid bodies where the motions of rigid bodies are known a priori, Glowinski, Pan and Périaux (1996) have coupled a time discretization by operator splitting à la Marchuk-Yanenko with a L^2-projection technique which forces the incompressibility condition; the resulting method is robust, stable and easy to implement.

With the help of those well-developed methodologies, we consider the numerical simulation of incompressible viscous flow around moving rigid bodies where the rigid body motions are caused by hydrodynamical forces and gravity; let us mention several applications, for examples, fluidized bed, sedimentation, blood flow around artificial heart valves. The method of choice is a *distributed Lagrange multiplier method* which consists to fill the moving bodies by the surrounding fluid and impose the rigid body motions to the fluid in the regions originally occupied by the rigid bodies; then we relax the rigid body motion constraint by using distributed Lagrange multipliers and obtain a flow problem over the entire region. The advantage of this approach is that we do not need to generate a new mesh each time right after finding the new position of the rigid bodies. This is a very important issue since for three dimensional particulate flows, generating meshes for simulating fluid-particle interactions is still a major difficulty and seems to require powerful parallel computers (see, e.g., Johnson & Tezduyar 1996). Through fictitious domain methods, we just need a very simple mesh for the particles which can be generated within seconds. Also we do not need to compute the hydrodynamical forces explicitly, since the interaction between fluid and particles is implicitly contained in the variational formulation. We have applied this approach to simulate the motion of sedimenting particles in a channel and captured the hydrodynamics interactions with the particles.

2. A MODEL PROBLEM AND ITS FICTITIOUS DOMAIN FORMULATION

With $B = B(t)$ a moving rigid particle ($B \subset \Omega \subset R^d$, $d = 2,3$) as in Figure 1, we consider for $t > 0$ the solution of the *Navier-Stokes equations*

$$\rho_f(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}) = \rho_f \mathbf{g} + \nabla\cdot\sigma \, in\, \Omega \setminus \overline{B(t)}, \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0 \, in\, \Omega\setminus\overline{B(t)}, \tag{2}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x}\in\Omega\setminus\overline{B(0)}, (with\, \nabla\cdot\mathbf{u}_0 = 0), \tag{3}$$

$$\mathbf{u} = \mathbf{g}_0 \, on\, \Gamma. \tag{4}$$

In (1)-(4) $\sigma = -p\mathbf{I} + \nu_f(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$ is the stress tensor, $\mathbf{u}$ and p denote as usual velocity and pressure, respectively; ρ_f is the density of the fluid, $\nu_f(>0)$ is the *viscosity*, $\mathbf{g}$ is the gravity, $\mathbf{x}$ the generic point of R^d ($\mathbf{x} = \{x_i\}_{i=1}^d$), $\Gamma_p(t) = \partial B(t)$, $\Gamma = \partial\Omega$, and $(\mathbf{u}\cdot\nabla)\mathbf{u} = \{\sum_{j=1}^{j=d} u_j \frac{\partial u_i}{\partial x_j}\}_{i=1}^{i=d}$. From the rigid body motion of the particle $B(t)$, $\mathbf{g}_0$ has to satisfy $\int_\Gamma \mathbf{g}_0\cdot\mathbf{n}\, d\Gamma = 0$ where $\mathbf{n}$ is the outer normal unit vector at Γ. In the following, we shall use, if necessary, the notation $\phi(t)$ for the function $\mathbf{x}\to\phi(\mathbf{x},t)$.

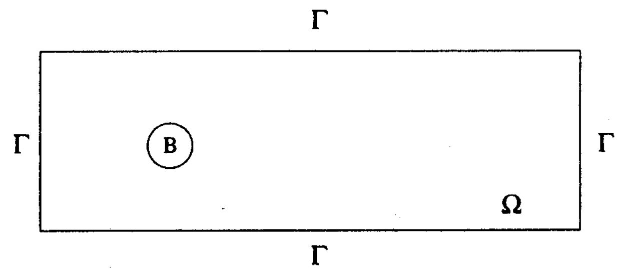

Figure 1. The flow region.

For simplicity we only consider the two-dimensional motion of a solid particle (we can easily extend the following approach to three-dimensional particle motion). By the Newton's law, we have

$$\frac{dV_p}{dt} = F_p + M\mathbf{g}, \quad I_p \frac{d\omega_p}{dt} = T_p, \quad \frac{dG_p}{dt} = V_p, \tag{5}$$

where V_p is the translation velocity of the particle, ω_p is the angular speed of the particle, M is the mass of the particle, I_p is the moment of inertia of the particle, G_p is the center of the particle, and g is the gravity. The force, F_p, and the moment, T_p, imposed on the particle by the fluid are given by

$$F_p = \int_{\Gamma_p(t)} \sigma \mathbf{n} \, d\Gamma, \qquad T_p = \int_{\Gamma_p(t)} (\mathbf{x} - G_p) \times (\sigma \mathbf{n}) \, d\gamma, \tag{6}$$

where $\mathbf{x}$ is the generic point of R^2 and $\mathbf{n}$ is the unit normal vector on the boundary of the particle pointing outward. The boundary condition on the boundary of the particle is

$$\mathbf{u} = V_p + \omega_p \times (\mathbf{x} - G_p), \ for\, \mathbf{x} \in \partial\Gamma_p(t). \tag{7}$$

To obtain a variational formulation for problem (1)-(7), we define the following spaces

$$\begin{aligned} \mathbf{V}_{\mathbf{g}_0(t)} = \{\mathbf{v} | \mathbf{v} \in H^1(\Omega \setminus \overline{B(t)})^2, \mathbf{v} = \mathbf{g}_0(t) \ on\, \Gamma, \\ \mathbf{v} = Y + \theta \times (\mathbf{x} - G_p) \ on\, \Gamma_p, \ Y \in R^2, \theta \in R\}, \end{aligned} \tag{8}$$

$$\begin{aligned} \mathbf{V}_0 = \{\mathbf{v} | \mathbf{v} \in H^1(\Omega \setminus \overline{B(t)})^2, \mathbf{v} = \mathbf{0} \ on\, \Gamma, \\ \mathbf{v} = Y + \theta \times (\mathbf{x} - G_p) \ on\, \Gamma_p, \ Y \in R^2, \theta \in R\}, \end{aligned} \tag{9}$$

$$L_0^2(\Omega \setminus \overline{B(t)}) = \{q | q \in L^2(\Omega \setminus \overline{B(t)}), \int_{\Omega \setminus \overline{B(t)}} q \, d\mathbf{x} = 0\}. \tag{10}$$

It can be show that the variational formulation of problem (1)-(7) is

For $t > 0$, *find* $\mathbf{u}(t) \in \mathbf{V}_{\mathbf{g}_0(t)}$, $p(t) \in L_0^2(\Omega \setminus \overline{B(t)})$, $(V_p(t), \omega_p(t)) \in R^3$, *such that*

$$\begin{cases} \rho_f \int_{\Omega \setminus \overline{B(t)}} \frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{v} \, d\mathbf{x} + \rho_f \int_{\Omega \setminus \overline{B(t)}} (\mathbf{u} \cdot \nabla)\mathbf{u} \cdot \mathbf{v} \, d\mathbf{x} - \int_{\Omega \setminus \overline{B(t)}} p \nabla \cdot \mathbf{v} \, d\mathbf{x} \\ +2\nu_f \int_{\Omega \setminus \overline{B(t)}} D(\mathbf{u}) : D(\mathbf{v}) \, d\mathbf{x} + Y \cdot (M \frac{dV_p}{dt} - M\mathbf{g}) + \theta I_p \frac{d\omega_p}{dt} \\ = \int_{\Omega \setminus \overline{B(t)}} \rho_f \mathbf{g} \cdot \mathbf{v} \, d\mathbf{x}, \ \forall \mathbf{v} \in \mathbf{V}_0, Y \in R^2, \ \theta \in R, \ a.e.\, t > 0, \end{cases} \tag{11}$$

$$\int_{\Omega \setminus \overline{B(t)}} q \nabla \cdot \mathbf{u}(t) \, d\mathbf{x} = 0, \ \forall q \in L^2(\Omega \setminus \overline{B(t)}), \tag{12}$$

$$\mathbf{u}(t) = V_p(t) + \omega_p(t) \times (\mathbf{x} - G_p(t)),\ for\, \mathbf{x} \in \partial\Gamma_p(t). \tag{13}$$
$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}),\ \mathbf{x} \in \Omega \setminus \overline{B(0)}, (with\, \nabla \cdot \mathbf{u}_0 = 0), \tag{14}$$
$$V_p(0) = V_p^0,\ \omega_p(0) = \omega_p^0. \tag{15}$$

where $D(\mathbf{v}) = (\nabla\mathbf{v} + (\nabla\mathbf{v})^T)/2$, $G_p(t) = G_p^0 + \int_0^t V_p(s)\, ds$, V_p^0 (resp., ω_p^0) is the initial velocity (resp., initial angular speed) of the particle $B(t)$ and G_p^0 is the initial center position of the particle (to our knowledge the variational formulation (11)-(15) was introduced by the second author in 1991).

Now we fill the moving rigid bodies $B(t)$ by the surrounding fluid (imbed $\Omega \setminus \overline{B(t)}$ in Ω) and impose the rigid body motions to the fluid in the regions originally occupied by the moving bodies. Then we relax the rigid body motion constraint by using distributed Lagrange multiplier and obtain a fictitious domain formulation over the entire region. Let us define the following spaces

$$\mathbf{W}_{\mathbf{g}_0(t)} = \{\mathbf{v} | \mathbf{v} \in H^1(\Omega)^2, \mathbf{v} = \mathbf{g}_0(t)\, on\, \Gamma\}, \quad \mathbf{W}_0 = H_0^1(\Omega)^2, \tag{16}$$
$$L_0^2(\Omega) = \{q | q \in L^2(\Omega), \int_\Omega q\, d\mathbf{x} = 0\}, \quad \Lambda(t) = L^2(B(t))^2,\ or\ H^1(B(t))^2, \tag{17}$$

and for $< \cdot, \cdot >_{B(t)}$, if $\Lambda(t) = L^2(B(t))^2$ we have

$$< \mu, \mathbf{v} >_{B(t)} = \int_{B(t)} \mu \cdot \mathbf{v}\, d\mathbf{x}, \forall \mu \in L^2(B(t))^2,\ \forall \mathbf{v} \in H^1(\Omega)^2; \tag{18}$$

if $\Lambda(t) = H^1(B(t))^2$, we have (for example)

$$< \mu, \mathbf{v} >_{B(t)} = \int_{B(t)} (\mu \cdot \mathbf{v} + \nabla\mu : \nabla\mathbf{v})\, d\mathbf{x}, \forall \mu \in H^1(B(t))^2,\ \forall \mathbf{v} \in H^1(\Omega)^2. \tag{19}$$

The fictitious domain formulation of problem (11)-(15) is

For $t > 0$, find $\mathbf{U}(t) \in \mathbf{W}_{\mathbf{g}_0(t)}$, $P(t) \in L_0^2(\Omega)$, $\lambda(t) \in \Lambda(t)$, $(V_p(t), \omega_p(t)) \in R^3$, such that

$$\begin{cases} \rho_f \int_\Omega \frac{\partial \mathbf{U}}{\partial t} \cdot \mathbf{v}\, d\mathbf{x} + \rho_f \int_\Omega (\mathbf{U} \cdot \nabla)\mathbf{U} \cdot \mathbf{v}\, d\mathbf{x} - \int_\Omega P \nabla \cdot \mathbf{v}\, d\mathbf{x} \\ +2\nu_f \int_\Omega D(\mathbf{U}) : D(\mathbf{v})\, d\mathbf{x} + (1 - \frac{\rho_f}{\rho_s}) M \frac{dV_p}{dt} \cdot Y + (1 - \frac{\rho_f}{\rho_s}) I_p \frac{d\omega_p}{dt} \theta \\ -(1 - \frac{\rho_f}{\rho_s}) M \mathbf{g} \cdot Y - < \lambda, \mathbf{v} - Y - \theta \times (\mathbf{x} - G_p) >_{B(t)} \\ = \int_\Omega \rho_f \mathbf{g} \cdot \mathbf{v}\, d\mathbf{x},\ \forall \mathbf{v} \in \mathbf{W}_0,\ Y \in R^2,\ \theta \in R,\ a.e.\, t > 0, \end{cases} \tag{20}$$

$$\int_\Omega q \nabla \cdot \mathbf{U}(t)\, d\mathbf{x} = 0,\ \forall q \in L^2(\Omega), \tag{21}$$
$$< \mu, \mathbf{U}(t) - V_p(t) - \omega_p(t) \times (\mathbf{x} - G_p(t)) >_{B(t)} = 0,\ \forall \mu \in \Lambda(t), \tag{22}$$
$$\mathbf{U}(\mathbf{x},0) = \mathbf{U}_0(\mathbf{x}),\ \mathbf{x} \in \Omega, (with\, \nabla \cdot \mathbf{U}_0 = 0), \tag{23}$$
$$\mathbf{U}(t) = \mathbf{g}_0(t),\ on\, \Gamma, \quad V_p(0) = V_p^0, \quad \omega_p(0) = \omega_p^0, \tag{24}$$

where $\mathbf{U}_0$ is an extension of $\mathbf{u}_0$ such that $\nabla \cdot \mathbf{U}_0 = 0$. Here we have $\mathbf{U}|_{\Omega\setminus\overline{B(t)}} = \mathbf{u}$ and $P|_{\Omega\setminus\overline{B(t)}} = p$. In (20), we can combine the gravity with pressure so in the following sections there is no gravity anymore.

3. FINITE ELEMENT APPROXIMATIONS

We still have that $\Omega \subset \boldsymbol{R}^2$. With h a *space discretization step* we introduce a finite element triangulation $\mathcal{T}_h$ of $\overline{\Omega}$ and then $\mathcal{T}_{2h}$ a triangulation twice coarser (in practice we should construct $\mathcal{T}_{2h}$ first and then $\mathcal{T}_h$ by joining the midpoints of the edges of $\mathcal{T}_{2h}$, dividing thus each triangle of $\mathcal{T}_{2h}$ into 4 similar subtriangles). We define then the following finite dimensional spaces which approximate $\mathbf{W}_{\mathbf{g}_0(t)}$, $\mathbf{W}_0$, $L^2(\Omega)$, $L^2_0(\Omega)$, respectively:

$$\mathbf{W}_{\mathbf{g}_{0h}} = \{\mathbf{v}_h | \mathbf{v}_h \in C^0(\bar{\Omega})^2,\ \mathbf{v}_h|_T \in P_1 \times P_1,\ \forall T \in \mathcal{T}_h,\ \mathbf{v}_h|_\Gamma = \mathbf{g}_{0h}\}, \tag{25}$$

$$\mathbf{W}_{0h} = \{\mathbf{v}_h | \mathbf{v}_h \in C^0(\bar{\Omega})^2,\ \mathbf{v}_h|_T \in P_1 \times P_1,\ \forall T \in \mathcal{T}_h,\ \mathbf{v}_h|_\Gamma = \mathbf{0}\}, \tag{26}$$

$$L^2_h = \{q_h | q_h \in C^0(\bar{\Omega}),\ q_h|_T \in P_1,\ \forall T \in \mathcal{T}_{2h}\},\ L^2_{0h} = \{q_h | q_h \in L^2_h,\ \int_\Omega q_h \, d\mathbf{x} = 0\}; \tag{27}$$

in (25), $\mathbf{g}_{0h}$ is an approximation of $\mathbf{g}_0$ satisfying $\int_\Gamma \mathbf{g}_{0h} \cdot \mathbf{n} \, d\Gamma = 0$.

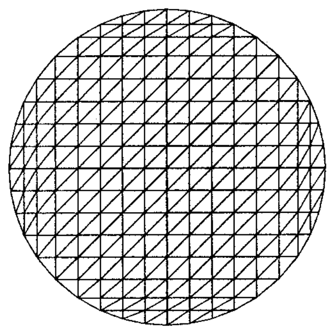

Figure 2. The triangulation of $\overline{B_h(t)}$ if $B(t)$ is a disk.

Let $\overline{B_h(t)}$ be a polygonal domain inscribed in $\overline{B(t)}$ and $\mathcal{T}_{B_h(t)}$ be a finite element triangulation of $\overline{B_h(t)}$ (see Figure 2). Then a finite dimensional space approximating $\Lambda(t)$ is

$$\Lambda_h(t) = \{\mathbf{v}_h | \mathbf{v}_h \in C^0(\overline{B_h(t)})^2,\ \mathbf{v}_h|_T \in P_1 \times P_1,\ \forall T \in \mathcal{T}_{B_h(t)}\}. \tag{28}$$

Using those finite dimensional spaces, we have

$$\begin{cases} \rho_f \int_\Omega \frac{\partial \mathbf{U}_h}{\partial t} \cdot \mathbf{v} \, d\mathbf{x} + \rho_f \int_\Omega (\mathbf{U}_h \cdot \nabla)\mathbf{U}_h \cdot \mathbf{v} \, d\mathbf{x} - \int_\Omega P_h \nabla \cdot \mathbf{v} \, d\mathbf{x} \\ +2\nu_f \int_\Omega D(\mathbf{U}_h) : D(\mathbf{v}) \, d\mathbf{x} + (1 - \frac{\rho_f}{\rho_s}) M \frac{dV_p}{dt} \cdot Y + (1 - \frac{\rho_f}{\rho_s}) I_p \frac{d\omega_p}{dt} \theta \\ -(1 - \frac{\rho_f}{\rho_s}) M\mathbf{g} \cdot Y - < \lambda_h, \mathbf{v} - Y - \theta \times (\mathbf{x} - G_p) >_{B_h(t)} \\ = 0,\ \forall \mathbf{v} \in \mathbf{W}_{0h},\ Y \in \boldsymbol{R}^2,\ \theta \in \boldsymbol{R},\ a.e.\ t > 0, \end{cases} \tag{29}$$

$$\int_\Omega q \nabla \cdot \mathbf{U}_h(t) \, d\mathbf{x} = 0,\ \forall q \in L^2_h, \tag{30}$$

$$< \mu, \mathbf{U}_h(t) - V_p(t) - \omega_p(t) \times (\mathbf{x} - G_p(t)) >_{B_h(t)} = 0,\ \forall \mu \in \Lambda_h(t), \tag{31}$$

$$\mathbf{U}_h(0) = \mathbf{U}_{0h},\ \mathbf{x} \in \Omega, \quad V_p(0) = V_p^0, \quad \omega_p(0) = \omega_p^0; \tag{32}$$

$$\{\mathbf{U}_h(t), P_h(t), \lambda_h(t), V_p, \omega_p\} \in \mathbf{W}_{\mathbf{g}_0(t)h} \times L^2_{0h} \times \Lambda_h(t) \times \boldsymbol{R}^3; \tag{33}$$

in (32), $\mathbf{U}_{0h}$ is an approximation of $\mathbf{U}_0$ so that $\int_\Omega q \nabla \cdot \mathbf{U}_{0h} \, d\mathbf{x} = 0$ for all $q \in L^2_h$.

4. TIME DISCRETIZATION BY OPERATOR SPLITTING

Most "modern" Navier-Stokes solvers are based on operator splitting algorithms in order to force the incompressibility condition via a Stokes solver or a L^2- projection method (see refs. Glowinski & Pironneau 1992 and Turek 1996 for details). This approach still applies to the initial value problem (29)-(33) which contains three numerical difficulties to each of which can be associated a specific operator, namely

1. The incompressibility condition and the related unknown pressure.
2. An advection-diffusion term.
3. The rigid body motion in $B_h(t)$ and the related multiplier $\lambda_h(t)$.

The operators in (1) and (3) are essentially *projection operators.* From an abstract point of view problem (29)-(33) is a particular case of the following class of initial value problems

$$\frac{d\phi}{dt} + A_1(\phi) + A_2(\phi) + A_3(\phi) = f,\ \phi(0) = \phi_0, \tag{34}$$

where the operators A_i can be *multivalued.* Among many operator splittings which can be employed to solve (34) we advocate the very simple one below (analyzed in, e.g., Marchuk 1990); it is only first order accurate but its low order accuracy is compensated by good stability and robustness properties.

A fractional step scheme à la Marchuk-Yanenko: With Δt a time discretization step and the initial guess, $\phi^0 = \phi_0$, the scheme is defined as follows

for $n \geq 0$, we obtain ϕ^{n+1} from ϕ^n via the solution of

$$(\phi^{n+j/3} - \phi^{n+(j-1)/3})/\Delta t + A_j(\phi^{n+j/3}) = f_j^{n+1}, \tag{35}$$

with $j = 1, 2, 3$ and $\sum_{j=1}^{3} f_j^{n+1} = f^{n+1}$. Applying scheme (35) to problem (29)-(33) we obtain (with $0 \leq \alpha, \beta \leq 1$, $\alpha + \beta = 1$ and after dropping some of the subscripts h):

$$\mathbf{U}^0 = \mathbf{U}_{0h};\ V_p^0,\ \omega_p^0, \text{ and } G_p^0 \text{ are given}; \tag{36}$$

for $n \geq 0$, knowing $\mathbf{U}^n$, V_p^n, ω_p^n, G_p^n, we compute $\mathbf{U}^{n+\frac{1}{3}}$, $P^{n+\frac{1}{3}}$ via the solution of

$$\begin{cases} \rho_f \int\limits_\Omega \dfrac{\mathbf{U}^{n+\frac{1}{3}} - \mathbf{U}^n}{\Delta t} \cdot \mathbf{v}\, d\mathbf{x} - \int\limits_\Omega P^{n+\frac{1}{3}} \nabla \cdot \mathbf{v}\, d\mathbf{x} = 0,\ \forall \mathbf{v} \in \mathbf{W}_{0h}, \\ \int\limits_\Omega q \nabla \cdot \mathbf{U}^{n+\frac{1}{3}}\, d\mathbf{x} = 0,\ \forall q \in L_h^2;\ \mathbf{W}^{n+\frac{1}{3}} \in \mathbf{W}_{\mathbf{g}_{0h}}^{n+1},\ P^{n+\frac{1}{3}} \in L_{0h}^2. \end{cases} \tag{37}$$

Then we compute $\mathbf{U}^{n+\frac{2}{3}}$, $V_p^{n+\frac{2}{3}}$, $G_p^{n+\frac{2}{3}}$ via the solution of

$$\begin{cases} \rho_f \int\limits_\Omega \dfrac{\mathbf{U}^{n+\frac{2}{3}} - \mathbf{U}^{n+\frac{1}{3}}}{\Delta t} \cdot \mathbf{v}\, d\mathbf{x} + 2\alpha\nu_f \int\limits_\Omega D(\mathbf{U}^{n+\frac{2}{3}}) : D(\mathbf{v})\, d\mathbf{x} \\ \quad + \rho_f \int\limits_\Omega (\mathbf{U}^{n+\frac{1}{3}} \cdot \nabla)\mathbf{U}^{n+\frac{2}{3}} \cdot \mathbf{v}\, d\mathbf{x} = 0,\ \forall \mathbf{v} \in \mathbf{W}_{0h}; \\ \mathbf{U}^{n+\frac{2}{3}} \in \mathbf{W}_{\mathbf{g}_{0h}}^{n+1}, \end{cases} \tag{38}$$

$$V_p^{n+\frac{2}{3}} = V_p^n + \mathbf{g}\Delta t, \quad G_p^{n+\frac{2}{3}} = G_p^n + (V_p^n + V_p^{n+\frac{2}{3}})\Delta t/2. \tag{39}$$

Finally we compute $\mathbf{U}^{n+1}$, λ^{n+1}, V_p^{n+1}, ω_p^{n+1}, G_p^{n+1} *via the solution of*

$$\begin{cases} \rho_f \int_\Omega \frac{\mathbf{U}^{n+1} - \mathbf{U}^{n+\frac{2}{3}}}{\Delta t} \cdot \mathbf{v}\,d\mathbf{x} + 2\beta\nu_f \int_\Omega D(\mathbf{U}^{n+\frac{2}{3}}) : D(\mathbf{v})\,d\mathbf{x} \\ +(1-\frac{\rho_f}{\rho_s})I_p \frac{\omega_p^{n+1} - \omega_p^n}{\Delta t}\theta + (1-\frac{\rho_f}{\rho_s})M\frac{V_p^{n+1} - V_p^{n+\frac{2}{3}}}{\Delta t} \cdot Y \\ =< \lambda_h, \mathbf{v} - Y - \theta \times (\mathbf{x} - G_p^{n+\frac{2}{3}}) >_{B_h^{n+\frac{2}{3}}}, \forall \mathbf{v} \in \mathbf{W}_{0h}, Y \in R^2, \theta \in R, \\ < \mu, \mathbf{U}^{n+1} - V_p^{n+1} - \omega_p^{n+1} \times (\mathbf{x} - G_p^{n+\frac{2}{3}}) >_{B_h^{n+\frac{2}{3}}} = 0, \forall \mu \in \Lambda_h^{n+\frac{2}{3}}; \\ \mathbf{U}^{n+1} \in \mathbf{W}_{\mathbf{g}_{0h}}^{n+1}, \lambda^{n+1} \in \Lambda_h^{n+\frac{2}{3}}, \end{cases} \tag{40}$$

$$G_p^{n+1} = G_p^n + (V_p^n + V_p^{n+1})\Delta t/2; \tag{41}$$

in (37)-(41) we have $\mathbf{W}_{\mathbf{g}_{0h}}^{n+1} = \mathbf{W}_{\mathbf{g}_0((n+1)\Delta t)h}$, $\Lambda_h^{n+1} = \Lambda_h((n+1)\Delta t)$, and $B_h^{n+s} = B_h((n+s)\Delta t)$. In (39) we predict the center of the particle location and use it in (40), then in (41) we correct the prediction of the center of the particle location.

5. SOLUTION OF SUBPROBLEMS (37), (38) AND (40)

By inspection of (37) it is clear that $\mathbf{U}^{n+1/3}$ is the $L^2(\Omega)^2$-projection of $\mathbf{U}^n$ on the (affine) subset of the functions $\mathbf{v} \in \mathbf{W}_{\mathbf{g}_{0h}}^{n+1}$ such that $\int_\Omega q\nabla\cdot\mathbf{v}\,d\mathbf{x} = 0$, $\forall q \in L_h^2$, $P^{n+1/3}$ being the corresponding Lagrange multiplier in L_{0h}^2. The pair $\{\mathbf{U}^{n+1/3}, P^{n+1/3}\}$ is *unique* and to compute it we can use an Uzawa/conjugate gradient algorithm operating in L_{0h}^2 equipped with the scalar product $\{q, q'\} \to \int_\Omega \nabla q \cdot \nabla q'\,d\mathbf{x}$. We obtained thus an algorithm preconditioned by the discrete equivalent of $-\Delta$ for the homogeneous Neumann boundary condition (Glowinski, Pan and Périaux 1996). Such an algorithm is *very* easy to implement and seems to have excellent convergence properties.

If $\alpha > 0$, problem (38) is a classical one; it can be easily solved, for example, by a least squares/conjugate gradient algorithm like those in Glowinski (1984).

The solution of problem (40) can be computed via algorithms similar to those for elliptic problems (Glowinski, Pan and Périaux 1994); except that here there are three more equations, the ones used to compute the translation velocity and angular speed of the particle. Problem (40) has the following form:

$$\begin{cases} \alpha \int_\Omega \mathbf{u}\cdot\mathbf{v}\,d\mathbf{x} + 2\nu \int_\Omega D(\mathbf{u}) : D(\mathbf{v})\,d\mathbf{x} \\ +(1-\frac{\rho_f}{\rho_s})I_p\frac{\omega_p - \omega_{p0}}{\Delta t}\theta + (1-\frac{\rho_f}{\rho_s})M\frac{V_p - V_{p0}}{\Delta t}\cdot Y \\ = \int_\Omega \mathbf{f}\cdot\mathbf{v}\,d\mathbf{x} + < \lambda_h, \mathbf{v} - Y - \theta \times (\mathbf{x} - G_p) >_{B_h}, \\ \forall \mathbf{v} \in \mathbf{W}_{0h}, Y \in R^2, \theta \in R, \\ < \mu, \mathbf{u} - V_p - \omega_p \times (\mathbf{x} - G_p) >_{B_h} = 0, \forall \mu \in \Lambda_h; \\ \mathbf{u} \in \mathbf{W}_{\mathbf{g}_{0h}}, \lambda \in \Lambda_h, \end{cases} \tag{42}$$

where the center G_p of particle B_h is known and $\mathbf{W}_{\mathbf{g}_{0h}} = \mathbf{W}^n_{\mathbf{g}_{0h}}$. A conjugate gradient algorithm for solving problem (42) is as follows:

Step 0: Initialization

$$\lambda_h^0 \in \Lambda_h \text{ is given;} \tag{43}$$

solve

$$\begin{cases} \alpha \int_\Omega \mathbf{u}^0 \cdot \mathbf{v}\, d\mathbf{x} + 2\nu \int_\Omega D(\mathbf{u}^0) : D(\mathbf{v})\, d\mathbf{x} \\ = \int_\Omega \mathbf{f} \cdot \mathbf{v}\, d\mathbf{x} + < \lambda_h^0, \mathbf{v} >_{B_h}, \ \forall \mathbf{v} \in \mathbf{W}_{0h};\ \mathbf{u}^0 \in \mathbf{W}_{\mathbf{g}_{0h}}, \end{cases} \tag{44}$$

$$(1 - \frac{\rho_f}{\rho_s}) M \frac{V_p^0 - V_{p0}}{\Delta t} \cdot Y = < \lambda_h^0, -Y >_{B_h}, \ \forall Y \in R^2, \tag{45}$$

$$(1 - \frac{\rho_f}{\rho_s}) I_p \frac{\omega_p^0 - \omega_{p0}}{\Delta t} \theta = < \lambda_h^0, -\theta \times (\mathbf{x} - G_p) >_{B_h}, \ \forall \theta \in R; \tag{46}$$

then

$$< \mu, \mathbf{g}^0 >_{B_h} = < \mu, \mathbf{u}^0 - V_p^0 - \omega_p^0 \times (\mathbf{x} - G_p) >_{B_h}, \ \forall \mu \in \Lambda_h, \tag{47}$$

and set

$$\mathbf{w}^0 = \mathbf{g}^0. \tag{48}$$

Then for $n \geq 0$, assuming that $\lambda_h^n, \mathbf{u}^n, V_p^n$, ω_p^n, $\mathbf{w}^n$, $\mathbf{g}^n$ are known we obtain λ_h^{n+1}, $\mathbf{u}^{n+1}$, V_p^{n+1}, ω_p^{n+1}, $\mathbf{w}^{n+1}$, $\mathbf{g}^{n+1}$ by

Step 1: Descent

Solve

$$\begin{cases} \alpha \int_\Omega \overline{\mathbf{u}}^n \cdot \mathbf{v}\, d\mathbf{x} + 2\nu \int_\Omega D(\overline{\mathbf{u}}^n) : D(\mathbf{v})\, d\mathbf{x} \\ = < \mathbf{w}^n, \mathbf{v} >_{B_h}, \ \forall \mathbf{v} \in \mathbf{W}_{0h};\ \overline{\mathbf{u}}^n \in \mathbf{W}_{0h}, \end{cases} \tag{49}$$

$$(1 - \frac{\rho_f}{\rho_s}) \frac{M}{\Delta t} \overline{V}_p^n \cdot Y = < \mathbf{w}^n, -Y >_{B_h}, \ \forall Y \in R^2, \tag{50}$$

$$(1 - \frac{\rho_f}{\rho_s}) \frac{I_p}{\Delta t} \overline{\omega}_p^n \theta = < \mathbf{w}^n, -\theta \times (\mathbf{x} - G_p) >_{B_h}, \ \forall \theta \in R; \tag{51}$$

and set

$$< \mu, \overline{\mathbf{g}}^n >_{B_h} = < \mu, \overline{\mathbf{u}}^n - \overline{V}_p^n - \overline{\omega}_p^n \times (\mathbf{x} - G_p) >_{B_h}, \ \forall \mu \in \Lambda_h. \tag{52}$$

Then we compute

$$\rho_n = < \mathbf{g}^n, \mathbf{g}^n >_{B_h} / < \mathbf{w}^n, \overline{\mathbf{u}}^n - \overline{V}_p^n - \overline{\omega}_p^n \times (\mathbf{x} - G_p) >_{B_h}, \quad (53)$$

and set

$$\lambda_h^{n+1} = \lambda_h^n - \rho_n w^n, \quad (54)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \rho_n \overline{\mathbf{u}}^n, \quad (55)$$

$$V_p^{n+1} = V_p^n - \rho_n \overline{V}_p^n, \quad (56)$$

$$\omega_p^{n+1} = \omega_p^{n+1} - \rho_n \overline{\omega}_p^n, \quad (57)$$

$$\mathbf{g}^{n+1} = \mathbf{g}^n - \rho_n \overline{\mathbf{g}}^n. \quad (58)$$

Step 2: Testing the convergence and construction of the new descent direction

If $< \mathbf{g}^{n+1}, \mathbf{g}^{n+1} >_{B_h} / < \mathbf{g}^0, \mathbf{g}^0 >_{B_h} \leq \epsilon$, *then take* $\mathbf{u} = \mathbf{u}^{n+1}$, $V_p = V_p^{n+1}$ *and* $\omega_p = \omega_p^{n+1}$. *If not, compute*

$$\gamma_n = < \mathbf{g}^{n+1}, \mathbf{g}^{n+1} >_{B_h} / < \mathbf{g}^n, \mathbf{g}^n >_{B_h}, \quad (59)$$

and set

$$\mathbf{w}^{n+1} = \mathbf{g}^n + \gamma_n \mathbf{w}^n. \quad (60)$$

Do $n = n + 1$ *and go back to* (49).

6. NUMERICAL EXPERIMENTS

The test problem that we consider concerns the simulation of the motion of two sedimenting cylinders in a channel of infinite length. The initial computational domain is $\Omega = (0, 2) \times (0, 15)$, then Ω is placed about 20 diameters ahead of the lower cylinder after the two cylinders are moving. The initial computational domain is $\Omega = (0, 2) \times (0, 15)$. The diameter of the cylinders is 0.25 cm and the centers are initially located at $(1, 5)$ and $(1, 5.5)$ respectivlely. Initial velocity and angular speed of the two cylinders are $V_p^0 = \mathbf{0}$, ω_p^0=0. The density of the fluid is $\rho_f = 1.0\, g/cm^3$ and the density of cylinders is $\rho_s = 1.01\, g/cm^3$. The viscosity of the fluid is $\nu_f = 0.01\, poise$. The initial condition for the fluid flow is $\mathbf{u} = \mathbf{0}$ and $\mathbf{g}_0(t) = \mathbf{0}$. The mesh size for the velocity field is $h_v = 1/50$ (there are 75851 nodes). The mesh size for pressure is $h_p = 1/25$ (19716 nodes). The time step is $\Delta t = 0.001$. The disk is cut into 368 triangles with 129 nodes (see Figure 2). We have chosen $\alpha = 1$ and $\beta = 0$ in the Marchuk-Yanenko scheme (36)-(41). With the finite dimensional spaces defined in (25)-(28), we have successfully captured the interactions between the two cylinders, i.e., drafting, kissing and tumbling (see Figure 3).

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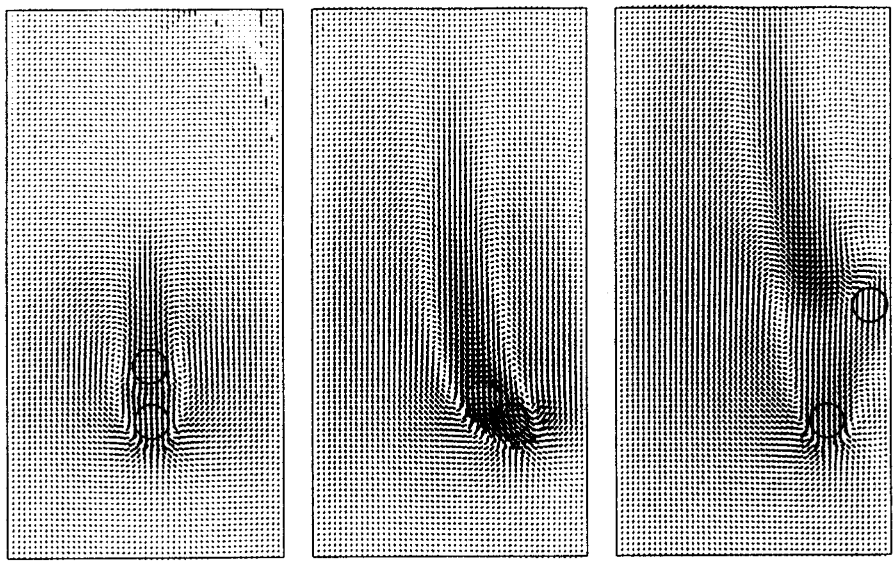

Figure 3. Drafting, kissing and tumbling of two sedimenting cylinders.

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