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Flow with suspended particles using fictitious domain and Lagrange multipliers: A fully implicit–fully coupled finite elements approach.

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Abstract. *Flows with suspended rigid particles occur in many different applications, from sedimentation problems to the manufacturing of ordered monolayer of micro and nano particles. The evolution of the particles position is a central point in the complete understanding of the flow of these suspensions. One way of analyzing the flow is to use a moving grid to discretize the Navier–Stokes equations that wraps around all suspended particles. This method requires remeshing and is not very efficient in the case of many particles. An alternative, that uses the fictitious domain approach, was first proposed by Glowinski et al (1999) [3] and later improved by Goano et al (2003) [2]. The Navier–Stokes equations are solved on a fixed grid and the particles move over this grid. Goano's approach avoids the need to grid around the rigid particles, solving the entire problem on a single fixed mesh. The Navier–Stokes equations are solved on the entire domain, but inside each particle, the flow is constrained to be a rigid body motion using Lagrange multipliers.*
This paper presents a fully implicit–fully coupled finite element formulation for the direct numerical simulation of incompressible fluid flows with suspended rigid particles based on the Lagrange multipliers/fictitious domain method. At each time step, the resulting non–linear system of equations is solved by Newton's method, with quadratic convergence which makes the iterative procedure very efficient to obtain the solution at each time step.
The method is validated using different test problems that simulate the sedimentation of one or more cylindrical particles in a box. The results obtained are compared with previous works, and the agreement is excellent.

Keywords: *Particulate Flows, Finite Elements, Fictitious Domain, Lagrange Multipliers*

1 INTRODUCTION

Particulate flows with small rigid particles suspended in a viscous fluid are found in many applications such as sedimentation, fluidized suspensions, slurries and coating and drying processes of micro and nano particles. The coupling between the suspending liquid flow and the particles motion is the central point in the complete understanding of the flow as in the sedimentation of a single particle at relatively high Reynolds number, shown in Figure 1.

Different numerical techniques have been developed over the years to model and simulate particle flows. In the first type of methods, the velocity and pressure fields of the fluid flow around each individual particle is determined by solving the Navier–Stokes system by some method of discretization, as finite element method in the work Hu et al (1992, 1996) [5, 4]. The hydrodynamic force acting on each particle is calculated from the fluid flow solution and is used on the movement equation. The finite element mesh has nodes over the fluid–solid boundaries, that moves with the particle. Therefore, a new mesh needs to be computed at each time step.

A second class of methods include what is called the fictitious domain method, proposed by Glowinski et al (1999) [3] and later improved by other works [1, 2, 6, 7, 8]. The entire domain, including fluid and particles, are discretized by the same mesh, and the Navier–Stokes equation is solved on the entire domain, but the velocity in the particle domain is constrained to have solid body motion. This approach eliminates the need for remeshing at every time step. Typically, the transient response is solved explicitly and an iterative procedure is used to solve the velocity and pressure field separately. The main contribution of this paper is to develop a fully implicit–fully coupled formulation for the numerical simulation of incompressible flows with suspended rigid particles. Our approach is based on the Lagrange multipliers/fictitious domain formulation proposed by Glowinski et al (1999) [3] and Goano et al (2003) [2], but avoids explicit projection methods and time–split integrators, solving at each time step the complete weak formulation through a single non–linear system of fully coupled equations. To solve the resulting non–linear system we use Newton's method. Since Newton's methods has quadratic convergence, only a few iterations are necessary to obtain the solution at each time step, which makes the method very efficient.

This work is presented using the following sections structure. In section 2 we will first review the governing equations of Newtonian incompressible fluids and solid rigid body particles and then derive the strong formulation for the particulate flow problem. In section 3 we will derive the finite elements formulation associated to the previously presented strong equations, and later describe the proposed fully implicit–fully coupled solver. In section 4 we will show numerical results and validations using different sedimentation test problems. Finally in section 5, we will discuss the conclusions obtained on this work and suggestions for possible directions to continue this work.

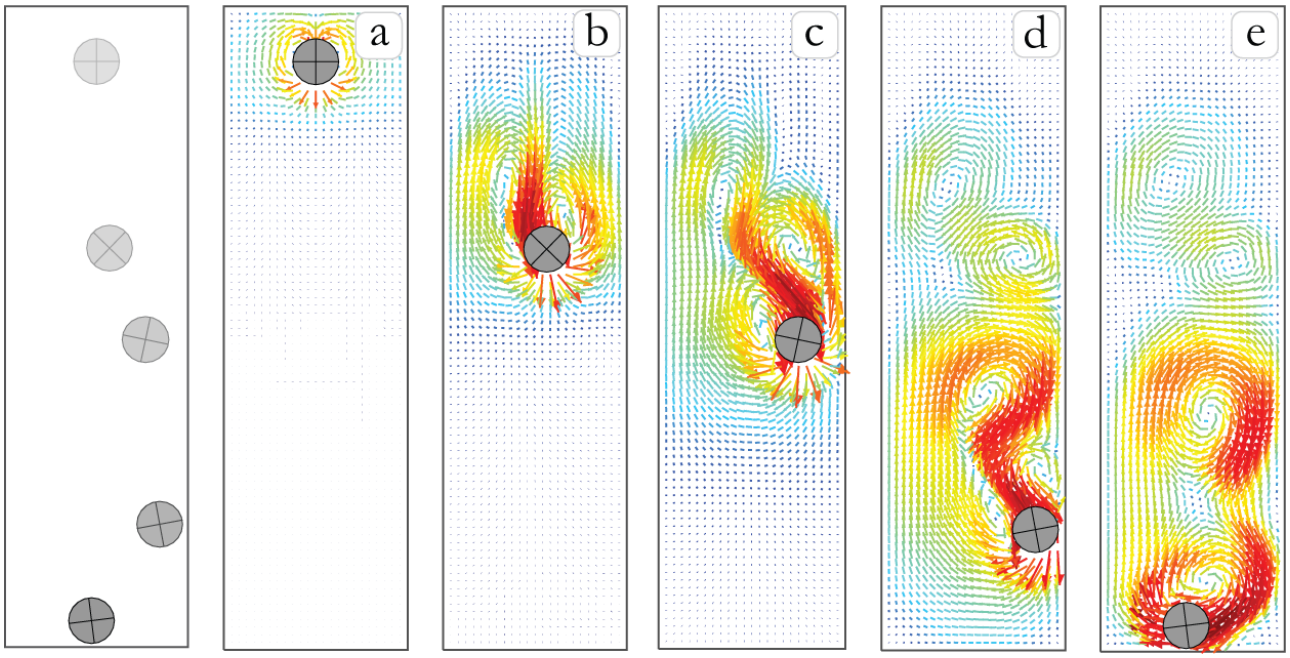

Figure 1. Single particle sedimentation: a particle of density 1.5 embedded on a incompressible fluid of viscosity 0.001 and density 1.0 falling under the gravity force.

2 A FICTITIOUS DOMAIN FORMULATION USING LAGRANGE MULTIPLIERS

The Lagrange multiplier/fictitious domain method for direct numerical simulation of incompressible flows with suspended particles was first proposed by Glowinski et al (1999) [3] and later improved by several works [1, 6, 7, 8] among them the paper of Goano et al (2003) [2]. The main advantage on the method of Glowinski is that the Navier–Stokes equations are solved on a fixed grid and the particles move over it. The Lagrange multipliers equations however, are solved in additional meshes built inside each particle. Goano's approach improves Glowinski's works avoiding the mesh inside the rigid particles, solving the entire problem on a single fixed grid. The Navier–Stokes equations are solved on the entire domain, but inside each particle, the flow is constrained to be a rigid body motion using Lagrange multipliers. Other key feature of the Lagrange multiplier/fictitious domain method is that the fluid–particle iteration is treated implicitly so no explicit calculation of the hydrodynamic forces and torque on particles is required.

The main goal of this section is to derive the strong formulation for the Lagrange multipliers based fictitious domain approach for the simulation of flows with suspended particles.

2 1 Governing Equations

Let us consider a bounded simulation domain Ω with external boundary $\partial\Omega$ filled with a fluid and embedded solid particles. We denote by Ω_f the region of Ω filled with a Newtonian fluid with density ρ_f and viscosity μ_f and by $\Omega_p = \bigcup_{i=1}^{n} \Omega_i$ the region of Ω filled with n rigid particles with densities ρ_i and radius R_i where $i \in \{1 \dots n\}$. Finally, let us represent the interface between the fluid and the particles by $\partial\Omega_p = \bigcup_{i=1}^{n} \partial\Omega_i$. Observe that $\Omega = \Omega_f \bigcup \Omega_p$ (see figure 2). The governing equations for the fluid in Ω_f are the Navier–Stokes equations:

$$\frac{\mathrm{D}(\rho_f \vec{u}_f)}{\mathrm{Dt}} = \nabla \cdot \boldsymbol{\sigma}_f \;\text{ and }\; \nabla \cdot \vec{u}_f = 0 \;\text{ in }\; \Omega_f \tag{1}$$

where $\vec{u}_f$ is the fluid's velocity, $\dfrac{\mathrm{D}*}{\mathrm{Dt}}$ denotes the material derivative and $\boldsymbol{\sigma}_f = -p_f\boldsymbol{\delta} + \mu_f(\nabla\vec{u}_f + \nabla\vec{u}_f^{\,t})$ is the stress tensor, p_f being the pressure in the fluid and $\boldsymbol{\delta}$ being the Identity tensor. Let us also denote the velocity of the centroid $\vec{X}_i$ of a particle p_i by $\vec{U}_i$ and its angular velocity by ω_i with $i \in \{1 \dots n\}$. The rigid-body motion equations of a solid particle are usually written as follows:

$$M_i \frac{\partial \vec{U}_i}{\partial t} = M_i\vec{g} + \vec{H}_i \;\text{ and }\; \mathbf{I}_i \frac{\partial \omega_i}{\partial t} + \omega_i \times \mathbf{I}_i\omega_i = \vec{T}_i \;\text{ in }\; \Omega_i \tag{2}$$

where M_i is the mass of the particle, $\vec{g}$ is the gravity acceleration, $\vec{H}_i$ is the hydrodynamic force acting on the particle, $\mathbf{I}_i$ is its inertial tensor and $\vec{T}_i$ is the hydrodynamic torque about its center of mass.

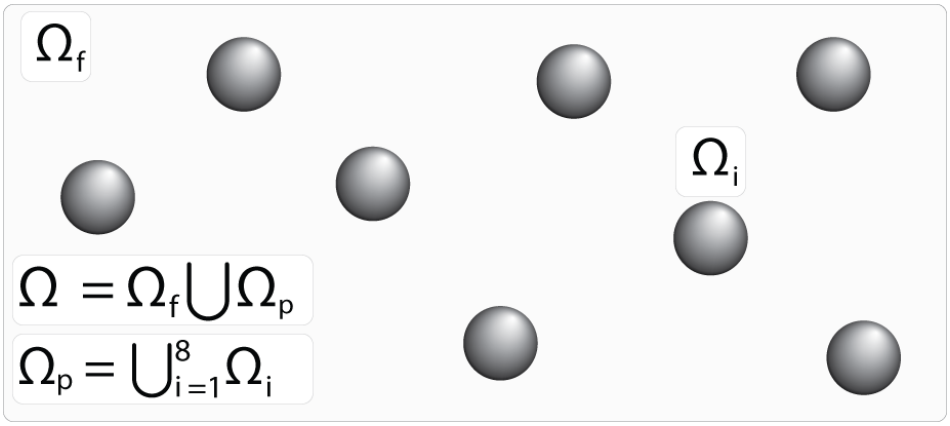

Figure 2. Simulation domain Ω: The fluid phase Ω_f and several particles covering the regions Ω_i.

2 2 Lagrange multipliers/fictitious domain formulation

The mathematical formulation of the proposed method is based on the formulation of Goano et al (2003) [2]. To start the derivation of the strong equations, let us define the velocity field $\vec{u}_p$ to be a rigid body velocity inside each particle and zero at the fluid region, i.e.:

$$\vec{u}_p = \begin{cases} \vec{U}_i + \omega_i \times (\vec{x} - \vec{X}_i) & \text{in } \Omega_i \text{ with } i \in (1 \dots n) \\ 0 & \text{in } \Omega_f \end{cases} \tag{3}$$

The momentum equation for $\vec{u}_p$ restricted on Ω_i can be written as follows:

$$\int_{\Omega_i} \frac{\mathrm{D}(\rho_i \vec{u}_p)}{\mathrm{Dt}} \, d\Omega_i = \int_{\Omega_i} (\rho_i - \rho_f)\vec{g} \, d\Omega_i + \int_{\partial\Omega_i} \vec{n}_i \cdot \boldsymbol{\sigma}_f \, d\partial\Omega_i \tag{4}$$

were $\vec{n}_i$ is the outward normal to $\partial\Omega_i$. It is important to notice that the surface integral term on the previous equation represents the total hydrodynamic force acting on the boundary of the particle p_i. Assuming that the stress tensor $\boldsymbol{\sigma}_f$ is Newtonian we can extended it over the entire domain Ω. Such extension can always be done if we define $\vec{u}$ and p as extensions over Ω of the velocity and pressure fields $\vec{u}_f$ and p_f satisfying $\vec{u}|_{\Omega_f} = \vec{u}_f$ and $p|_{\Omega_f} = p_f$. Using the divergence theorem and the extended stress tensor $\boldsymbol{\sigma} = -p\boldsymbol{\delta} + \mu_f(\nabla\vec{u} + \nabla\vec{u}^t)$, we can rewrite equation 4 as :

$$\int_{\Omega_i} \frac{\mathrm{D}(\rho_i \vec{u}_p)}{\mathrm{Dt}} \, d\Omega_i = \int_{\Omega_i} (\rho_i - \rho_f)\vec{g} \, d\Omega_i + \int_{\Omega_i} \nabla \cdot \boldsymbol{\sigma} \, d\Omega_i \tag{5}$$

Now, let us adopt the following notation:

$$\vec{F} = \begin{cases} -\dfrac{\mathrm{D}(\rho_f \vec{u})}{\mathrm{Dt}} + \nabla \cdot \boldsymbol{\sigma} & \text{in } \Omega_p \\ 0 & \text{in } \Omega_f \end{cases} \tag{6}$$

If we impose an additional constraint to the extended velocity field $\vec{u}$ that states $\vec{u} = \vec{u}_p$ in Ω_i, the momentum equation for the particle p_i becomes:

$$\int_{\Omega_i} \frac{\mathrm{D}[(\rho_i - \rho_f)\vec{u}]}{\mathrm{Dt}} \, d\Omega_i = \int_{\Omega_i} [(\rho_i - \rho_f)\vec{g} + \vec{F}] \, d\Omega_i \tag{7}$$

It is very important to observe that we can interpret the additional force per unit volume $\vec{F}$ in the previous momentum equation, as the interaction force between the fluid and particle phases. Moreover, as we will see in the following it enforces the rigid body motion onto the fluid velocity field within each of the particles.

From the previous equation, observing that $\vec{u}$ is a rigid body velocity inside each particle p_i, we can write the equation that describes the particle's velocity $\vec{U}_i$ as follows:

$$\Delta M_i \frac{\partial \vec{U}_i}{\partial t} = \Delta M_i \vec{g} + \int_{\Omega_i} \vec{F} \, d\Omega_i \tag{8}$$

where $\Delta M_i = \int_{\Omega_i} (\rho_i - \rho_f)\, d\Omega_i$. Moreover, we can recover the angular velocity ω_i from the no–slip boundary condition on the surface of particle p_i. After some algebraic manipulation and using the Stokes theorem, yields that:

$$\omega_i V_i = \frac{1}{2}\int_{\Omega_i} \nabla \times (\vec{u} - \vec{U}_i)\, d\Omega_i \tag{9}$$

where V_i is the volume of the particle p_i. Using the force $\vec{F}$ between the phases, the extended velocity $\vec{u}$ and pressure p fields and stress tensor $\boldsymbol{\sigma}$, we can rewrite the equations of motion on the fluid phase (equation 1) as follows:

$$\frac{\mathrm{D}(\rho_f \vec{u})}{\mathrm{Dt}} = \nabla \cdot \boldsymbol{\sigma} - \vec{F} \ \text{ and } \ \nabla \cdot \vec{u} = 0 \ \text{ in } \quad \Omega \tag{10}$$

As we observed before, it is clear now from equations 8 and 10 that $\vec{F}$ is a term that enforces the rigid–body constraint onto the field $\vec{u}$ inside each particle p_i. It is non–zero only within the domain of the particles Ω_p however, its impact on the fluid's velocity is over the entire domain, due to equation 10. Following the approach of Goano et al (2003) [2], we can now define a global Lagrange multiplier $\vec{\lambda}$ which is related to $\vec{F}$ through the following boundary value problem:

$$\vec{F} = -\alpha\vec{\lambda} + \mu_f \triangle\vec{\lambda} \ \text{ in } \ \Omega \ \text{ and } \ \vec{\lambda} = 0 \ \text{ on } \ \partial\Omega \tag{11}$$

where α is a positive constant parameter. The problem defined by equation 11 is a well posed problem for $\vec{F}$ and it is more efficient to use its unique solution to impose the rigid–body constraint on the extended velocity field $\vec{u}$. Notice that $\vec{\lambda}$ has the same regularity of $\vec{u}$. Observe also that the Lagrange multipliers field is non–zero only inside the particles domain, and we can require $\vec{\lambda}$ to be zero on the fluid domain, that is $\vec{\lambda} = 0 \ \text{ in } \ \Omega_f$.

Finally, the strong formulation of the particulate flows governing equations that will be used further to compute the extended velocity $\vec{u}$ and pressure p, the particle's velocity $\vec{U}_i$ and angular velocity ω_i can be written as follows:

$$\begin{aligned}
&\frac{\mathrm{D}(\rho_f \vec{u})}{\mathrm{Dt}} = \nabla \cdot \boldsymbol{\sigma} + \alpha\vec{\lambda} - \mu_f \triangle\vec{\lambda} \ \text{ and } \ \nabla \cdot \vec{u} = 0 && \text{in } \ \Omega \\
&\Delta M_i \frac{\partial \vec{U}_i}{\partial t} = \Delta M_i \vec{g} - \int_{\Omega_i} \alpha\vec{\lambda}\, d\Omega_i - \mu_f \int_{\partial\Omega_i} \nabla\vec{\lambda}\vec{n}_i\, d\partial\Omega_i && \text{with } \ i \in (1 \ldots n) \\
&\omega_i V_i = \frac{1}{2}\int_{\Omega_i} \nabla \times (\vec{u} - \vec{U}_i)\, d\Omega_i && \text{with } \ i \in (1 \ldots n)
\end{aligned} \tag{12}$$

Notice that the second equation is the same written in equation 8 but we have integrated $\triangle\vec{\lambda}$ by parts. In addition to the system of equations 12 the rigid body and the Lagrange multipliers constraint equations must be included in the complete strong formulation even as the particle advection equation:

$$\begin{aligned}
&\vec{\lambda} = 0 && \text{in } \ \Omega_f \\
&\vec{u} = \vec{U}_i + \omega_i \times (\vec{x} - \vec{X}_i) && \text{in } \ \Omega_i \\
&\frac{\partial \vec{X}_i}{\partial t} = \vec{U}_i && \text{with } \ i \in (1 \ldots n)
\end{aligned} \tag{13}$$

3 A FULLY IMPLICIT–FULLY COUPLED FINITE ELEMENTS APPROACH

The previous works on direct numerical simulation of flows with suspended particles that uses the Lagrange multipliers/fictitious domain approach [1, 2, 3, 6, 7, 8] solve the non–linear system of equations 12 and 13 using finite–elements method together with time–discretization approach based on Navier–Stokes projection schemes and additional iterations for imposing the rigid–body constraint. The main disadvantage of these methods is that they are uncoupled and explicit integrators for time–variable differential equations that suffers from well known problems such as loss of accuracy and numerical instabilities.

In this work, a fully implicit–fully coupled finite elements solver is proposed for Lagrange multipliers/fictitious domain based numerical simulation of flows with suspended particles. By *"fully implicit–fully coupled"* we mean that we use a implicit time integration and that at each time step, a single coupled system of non–linear equations that comes from the finite elements space discretization and from the implicit Euler time integration is solved by Newton's method, which has quadratic convergence and makes the iterative procedure very efficient.

3 1 Finite elements discretization

In the Lagrange multipliers/fictitious domain method the computational domain Ω is discretized by means of a single and fixed finite element mesh. To write the equations stated on the strong formulation (equations 12 and 13) in a finite element form, we will need to derive a Garlekin weak formulation. The mathematical argumentation in the previous section is based on the fact that the velocity field $\vec{u}$ is constrained to be a rigid–body motion inside de particle domain Ω_p. So a natural choice for the combined solution space for the fluid and particle velocities and for the fluid pressure is:

$$\mathbb{C} = \{(\vec{u}, p, \vec{U}_i, \omega_i) | \vec{u} \in \mathbb{H}^1(\Omega), p \in \mathbb{H}^0(\Omega), \vec{U}_i \in \mathbb{R}^2 \text{ and } \omega_i \in \mathbb{R} \text{ with } \vec{u} = \vec{U}_i + \omega_i \times (\vec{x} - \vec{X}_i),\ i \in (1 \dots n)\} \quad (14)$$

From the combined solution space, we can give a different interpretation for the previous strong formulation (equations 12 and 13). In our Lagrange multiplier approach the extended formulation over the whole domain is obtained removing the fluid's velocity restriction $\vec{u} = \vec{U}_i + \omega_i \times (\vec{x} - \vec{X}_i)$ from the combined solution space, and enforcing it as a side constraint. As we saw before, this is done using the Lagrange multipliers $\vec{\lambda}$, which can also be interpreted as the traction force required to maintain the rigid–body motion in each particle domain Ω_i. The last two equations in the strong formulation of the governing equations (equations 12) are a differential and an algebraic equation respectively that are used to determine the unknowns $\vec{U}_i$ and ω_i and therefore they must be incorporated into the final weak form without additional mathematical manipulations.

Now let us denote by $\vec{\phi} = \sum_i c_i \vec{\phi}_i \in \mathbb{H}^1(\Omega)$ and $\chi = \sum_j \overline{c}_j \chi_j \in \mathbb{H}^0(\Omega)$ two arbitrary fields in their respective Sobolev spaces, where $\vec{\phi}_i$ and χ_j are basis of $\mathbb{H}^1(\Omega)$ and $\mathbb{H}^0(\Omega)$ respectively. After some algebraic manipulation of the extended stress tensor and the Lagrange multiplier laplacian on the Navier–Stokes momentum equation, the full weak formulation can be written as:

Find $\vec{u} \in \mathbb{H}^1(\Omega)$, $\vec{\lambda} \in \mathbb{H}^1(\Omega)$, $p \in \mathbb{H}^0(\Omega)$, $\omega_i \in \mathbb{R}$ and $\vec{U}_i \in \mathbb{R}^2$ such that $\forall \vec{\phi} \in \mathbb{H}^1(\Omega)$ and $\forall \chi \in \mathbb{H}^1(\Omega)$:

$$\begin{aligned}
&\int_\Omega \rho_f \frac{\mathrm{D}\vec{u}}{\mathrm{Dt}} \cdot \vec{\phi}\, d\Omega = \int_\Omega (\alpha \vec{\lambda} \cdot \vec{\phi} - \boldsymbol{\sigma} : \nabla \vec{\phi} + \mu_f \nabla \vec{\lambda} : \nabla \vec{\phi})\, d\Omega + \int_{\partial\Omega} (\vec{n} \cdot \boldsymbol{\sigma} - \mu_f \nabla \vec{\lambda} \cdot \vec{n}) \cdot \vec{\phi}\, d\partial\Omega \qquad \text{in } \Omega \\
&\int_\Omega (\nabla \cdot \vec{u}) \chi\, d\Omega = 0 \qquad \text{in } \Omega \\
&\int_{\Omega_f} \vec{\lambda} \cdot \vec{\phi}\, d\Omega_f = 0 \qquad \text{in } \Omega_f \\
&\int_{\Omega_i} \vec{u} \cdot \vec{\phi}\, d\Omega_i = \int_{\Omega_i} [\vec{U}_i + \omega_i (\vec{x} - \vec{X}_i)] \cdot \vec{\phi}\, d\Omega_i = 0 \qquad \text{with } i \in (1 \dots n) \\
&\Delta M_i \frac{\partial \vec{U}_i}{\partial t} = \Delta M_i \vec{g} - \int_{\Omega_i} \alpha \vec{\lambda}\, d\Omega_i - \mu_f \int_{\partial\Omega_i} \nabla \vec{\lambda} \cdot \vec{n}_i\, d\partial\Omega_i \qquad \text{with } i \in (1 \dots n) \\
&\omega_i V_i = \frac{1}{2} \int_{\Omega_i} \nabla \times (\vec{u} - \vec{U}_i)\, d\Omega_i \qquad \text{with } i \in (1 \dots n)
\end{aligned} \quad (15)$$

where $\vec{n}$ represents the outward normal to $\partial\Omega$. As you can see, the momentum and the continuity Navier–Stokes equations are defined over the hole domain Ω, and that is the reason why this weak formulation can be solved on a single and fixed discretization of Ω, avoiding the need of remeshing around the particles.

We used quadrangular $\mathbb{P}_2$–$\mathbb{P}_1$ elements, which have continuous bilinear interpolation for the velocity $\vec{u}$ and the Lagrange multipliers $\vec{\lambda}$ fields, and continuous linear interpolations for the pressure p. It is well known that quadrangular $\mathbb{P}_2$–$\mathbb{P}_1$ elements are stable basis functions for solving the Navier–Stokes equations using the finite elements method and for this reason we also adopted it on our particulate flow application.

We perform the integrations that appear on the weak formulation using the Gaussian Quadrature method, which has very good accuracy. However, a special attention is necessary when computing the integrals over each particle domain, since Ω_i in general it is not exactly covered with finite elements. In case that the surface of the particle intersects the interior of a given element, we can choose to perform one of two solutions: the first approach consider only the Gaussian points that lies inside the particle p_i to perform the integration over Ω_i, and the second solution virtually adapts the mesh around the particle, that is, the mesh refinement is done without changes on the original mesh. The first approach was the integration correction used on the results that will be presented on the next section. This choice was based on the ease and efficiency of implementation if compared with the subdivision approach. Despite being the less accurate solution, our results shows that this scheme works nicely.

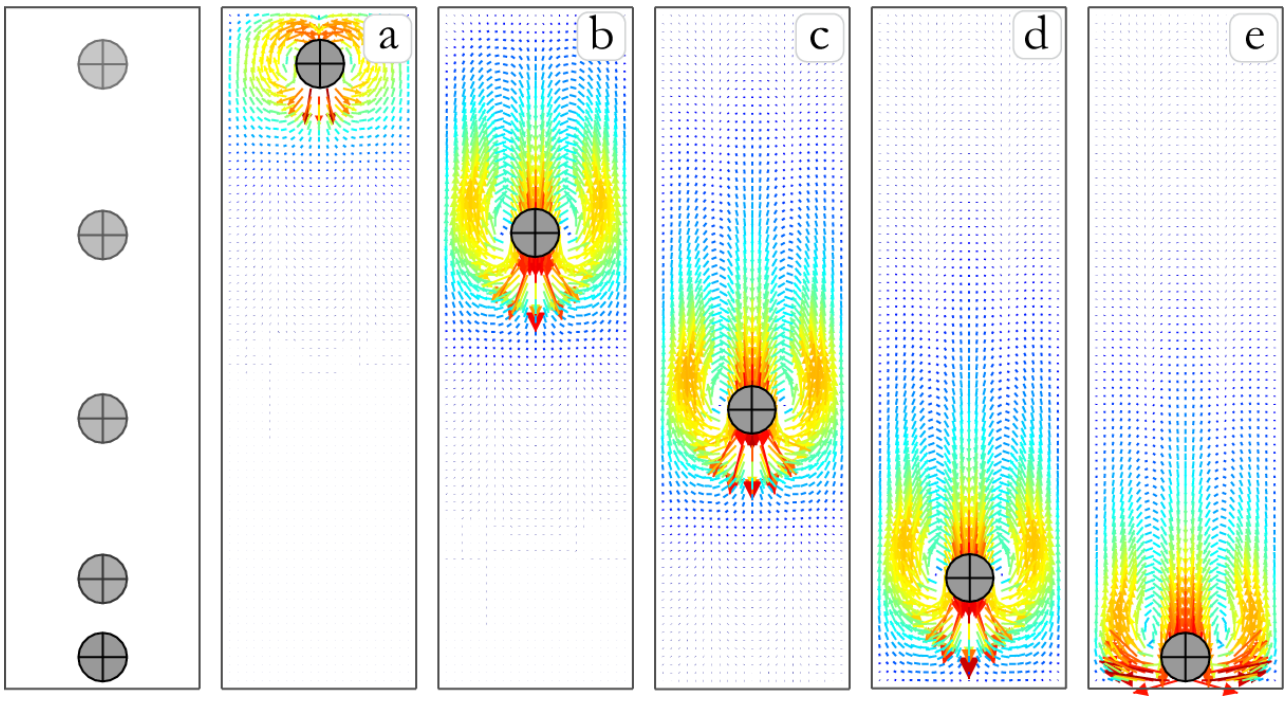

Figure 3. Single particle sedimentation: a particle of density 1.8 embedded on a incompressible fluid of viscosity 0.01 and density 1.0 falling under the gravity force.

3 2 Fully implicit–fully coupled solver

Observe that, at each time step, the weak formulation (equation 15) leads to a system of non–linear time–variable differential equations. In our formulation, we used an implicit Euler method as time integrator because in many cases, the problems arising from particulate flow applications are stiff and the use of an explicit method requires impractically small time steps Δt to keep the error in the result bounded. For such problems, to achieve a given accuracy, it takes much less computational time to use an implicit method with larger time steps.

While explicit methods compute the physical unknowns at a later time using the solution obtained at the current time, an implicit method finds it by solving an equation involving both the current solution and the later time unknowns. Mathematically, if $s^{(t)}$ is the current solution and $s^{(t+1)}$ is the physical unknowns at the later time, then for an implicit method:

$$\frac{\partial \vec{s}}{\partial t} = f(t, \vec{s}) \implies \frac{\vec{s}^{(t+1)} - \vec{s}^{(t)}}{\Delta t} = f(t, \vec{s}^{(t+1)}) \implies \vec{s}^{(t)} = \vec{s}^{(t+1)} - f(t, \vec{s}^{(t+1)})\Delta t \tag{16}$$

which clearly indicates that we must solve a system of equations to obtain the physical values at the later time $s^{(t+1)}$. The momentum equation of the Navier–Stokes equations is a non–linear equation for the extended fluid velocity $\vec{u}$, and consequently the system of equations of the implicit Euler formulation is in fact a non–linear system of equations.

We solved the weak formulation of equation 15 and the implicit Euler time integration in a single and fully coupled system of non–linear equations, using Newton's method. Newton's method is an extremely powerful and fast iterative technique since it has in general quadratic convergence, i.e., the error is essentially squared at each iteration. The method's algorithm requires the construction of the Jacobian matrix $\mathbf{J}$ and of the residue vector $\vec{r}$ associated to the system at each iteration of the procedure. Intuitively the Jacobian's matrix can be thought as the sensibility of each equation in relation to each problem's unknown.

Algorithm 1 Newton's method iterative procedure

$\vec{U}^{(t+1)} \leftarrow (x_1^{(0)}, x_2^{(0)}, x_3^{(0)}, \ldots, x_k^{(0)})$ // Initial guess.
while $|\vec{U}^{(t+1)} - \vec{U}^{(t)}| < \epsilon$ **do**
  $\mathbf{J}(\Delta\vec{U}^{(t+1)}) = -\vec{r}(\vec{U}^{(t)})$
  $\vec{U}^{(t+1)} = \vec{U}^{(t)} + \Delta\vec{U}^{(t+1)}$
end while

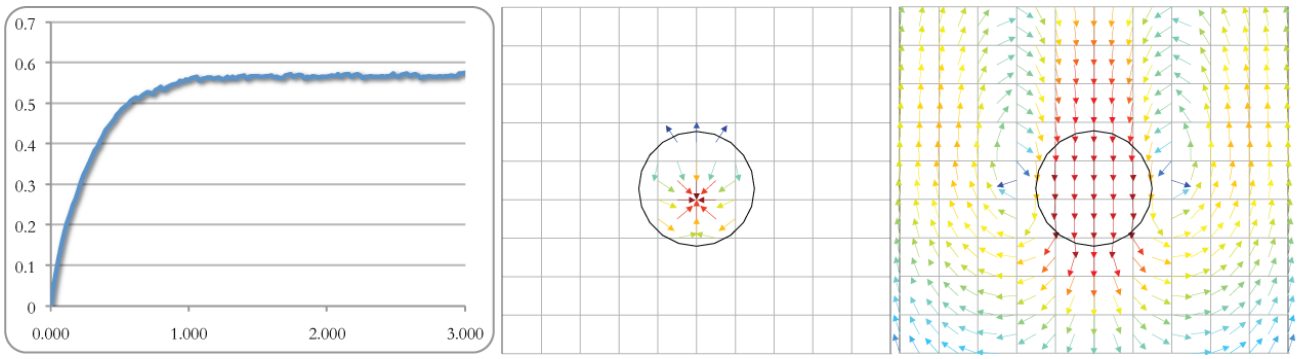

Figure 4. In the image on left we can see the variation of the particle's velocity in the first three seconds of the simulation. In the other two images we can see the Lagrange multipliers and the constrained velocity field inside the rigid particle at a given frame. All images are obtained from to the single particle sedimentation test case.

In Newton's method, the update vector is obtained by solving a linear system of equations defined by the Jacobian matrix and by the residue vector at each iteration. In finite element applications this system is usually sparse, and may require the use of sparse iterative linear algebra algorithms. Newton's method for solving a non–linear system of equation can be implemented using the procedure described in algorithm 1.

Observe that the algorithm 1 requires an initial guess to start the iterative procedure. If the given initial value is too far from the true zero, Newton's method may fail to converge. For this reason, Newton's method is often referred to as a local technique. There are several techniques that help to find good initial guesses. The initial guess at each time step was obtained by a linear extrapolation of the two previous time steps.

4 NUMERICAL RESULTS

In this section, we will show several results obtained by the Lagrange multipliers/fictitious domain method proposed in this work. We validated our implementation by comparing the results in different test problems that simulate the fluid–particle iteration for one or more cylindrical particles in a box. The agreement was excellent.

For all results presented on this section, we included one figure (that is the composition of six images) illustrating the test case dynamics. The first image in each figure is the overlap of the particle's position obtained from five chosen key frames of the simulation. The images from (a) to (e) are the full representation of each key frames and includes also the fluid's velocity field representation. As we can see, the fluid's velocity are colored according with its magnitude. In all images, we can observe a cross mark inside each particle. The cross mark helps us to visualize the angular orientation of the particles during the simulation.

4 1 Single particle sedimentation

The first example is the sedimentation of one particle in a box. The results are shown in figure 3. The complete set of parameters is the following: the domain Ω is a closed box with dimensions $[-0.286, 0.286] \times [-1.0, 1.0]$, discretized by a mesh of 504 squared elements with $\mathbb{P}_2$–$\mathbb{P}_1$ finite elements basis functions. The fluid phase Ω_f is a Newtonian incompressible fluid with density $\rho_f = 1.0$. The fluid's viscosity is $\mu_f = 0.01$. A single cylindrical particle with radius $R_p = 0.0714$ and density $\rho_p = 1.8$ is embedded on the fluid. The particle is initially on rest and at position $\vec{X}_p = (0.869, 0)$. The simulation's time step is δt $= 0.02$ seconds and the total simulated time is 13 seconds. Finally, following the work of Goano et al (2003)[2], we set the Lagrange multiplier parameter α to be 75.

Figure 4(a) shows the evolution of the particle velocity and the result can be compared with the well known study case of the flow over a fixed cylinder. The terminal velocity of of a cylinder falling in a box can be evaluated based on a drag force acting on the cylinder. For $\rho_p = 1.8$, the terminal velocity obtained by an asymptotic solution is $\vec{U}_t = 0.593$. In our implementation, the computed final velocity tends to $\vec{U}_t^* = 0.575$.

The example shown in figure 1 as a motivation, clearly shows the coupling between the flow and the particle dynamics. The problem is the same as the one presented in Figure 3, the only difference is the fluid viscosity $\mu_f = 0.01$. With the lower fluid viscosity, the particle velocity is higher and so is the Reynolds number of the flow. A periodic flow motion develops in the wake of the cylinder as the result of the Karman vortices. The asymmetry of the flow is clear in Figure 1(c). In this case, the particle does not fall vertically.

As we showed during the derivation of the method's formulation, the Lagrange multipliers imposes the rigid body constraint to the fluid's velocity onto the particle's region Ω_p. The last two images of figure 4, shows the Lagrange multipliers and the constrained velocity field solution obtained by our software on the instant illustrated by the image

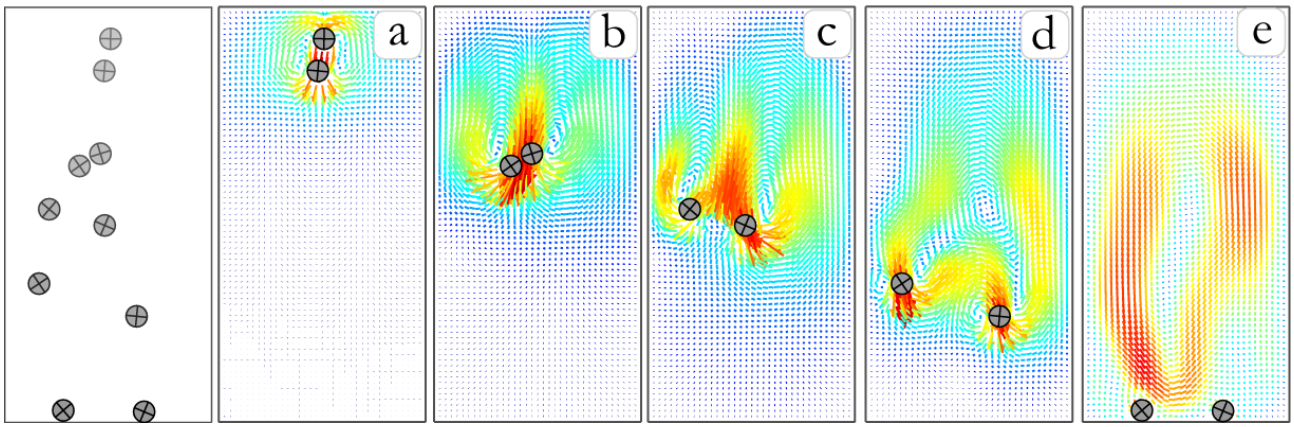

Figure 5. Two particles sedimentation: two particle of density 1.5 embedded on a incompressible fluid of viscosity 0.01 and density 1.0 falling under the gravity force. We can observe the simulation reproduces the particles iteration dynamics usually called drafting, kissing and tumbling.

(c) on the single particle sedimentation test case showed in figure 3. Notice that the solution is symmetric along a vertical passing through the center of the particle, and this behavior keeps the angular orientation unchanged during all the simulation. In this figure, the Lagrange multipliers fields are normalized for better visualization, and they are colored, from blue to red, according their magnitude. The gray circle shows the boundary of the particle's domain.

4 2 Two particles sedimentation – drafting, kissing and tumbling

The next test problem is the simulation of the sedimentation of two cylindrical particles (see figure 5). The complete set of parameters for the simulation is the following: the domain Ω is a closed box with dimensions $[-0.5, 0.5] \times [-1.0, 1.0]$, discretized by a mesh of 666 squared elements with $\mathbb{P}_2$–$\mathbb{P}_1$ finite elements basis functions. The fluid phase Ω_f is a Newtonian incompressible fluid with density $\rho_f = 1.0$ and viscosity is $\mu_f = 0.01$. Two cylindrical particles with radius $R_{1,2} = 0.0514$ and density $\rho_{1,2} = 1.8$ are embedded on the fluid. The particles are initially on rest and at position $\vec{X}_1$ = $(0.015, 0.9)$ and $\vec{X}_2$ = $(-0.015, 0.75)$. The simulation's time step is δt $= 0.02$ seconds and the total simulated time is 7 seconds. Again, we set the Lagrange multiplier parameter α to be 75, following the work of Goano et al (2003)[2].

Particle pair interactions are fundamental mechanisms, which enter strongly into all practical applications of particulate flows. They are due to inertia and normal stresses. The principal interactions between neighboring cylindrical particles in Newtonian liquids can be described as drafting, kissing and tumbling. When one falling cylinder enters the wake of another, it experiences reduced drag, drafts downward toward the leading particle, and kisses it. The two kissing particles momentarily form a single long body aligned parallel to the stream. But the parallel orientation for a falling long body is unstable and the pair of kissing particles tumbles to a side-by-side configuration. Two touching particles falling side-by-side are pushed apart until a stable separation distance between centers across the stream is established; they then fall together without further lateral migrations. This dynamics can be easily observed on the figure 5.

4 3 Single particle dragged by the fluid

The last result shows the motion of one cylindrical particle lighter than the fluid that is being dragged by the flow inside a lid–driven cavity (see figure 6). The lid–driven cavity problem has long been used as a test or validation case for new codes or new solution methods because the problem geometry is simple and two-dimensional, the boundary conditions are also simple and the flow is quite complex with the presence of recirculations. The standard case is a fluid contained in a square domain with Dirichlet boundary conditions on all sides, with three stationary sides and one moving side (with velocity tangent to the side). In our approach a solid cylindrical particle is also embedded on the fluid.

The complete set of parameters for the simulation is the following: the domain Ω is a closed box with dimensions $[-1.0, 1.0] \times [-0.25, 0.25]$ which lid moves with velocity $\vec{u}_l = (1, 0)$, and discretized by a mesh of 400 squared elements with $\mathbb{P}_2$–$\mathbb{P}_1$ finite elements basis functions. The fluid phase Ω_f is a Newtonian incompressible fluid with density $\rho_f = 1.0$ and viscosity is $\mu_f = 0.01$. One cylindrical particle with radius $R_p = 0.0714$ and density $\rho_p = 0.65$ is embedded on the fluid. The particle is initially on rest and at position $\vec{X}_p$ = $(0.0, 0.1786)$. The simulation's time step is δt $= 0.02$ seconds and the total simulated time is 7 seconds. The Lagrange multiplier parameter α is set to value 75.

When the particle is lighter than the fluid, it moves upwards and it ends up near the upper right corner of the cavity as shown in the right column of figure 6. When the particle density is $\rho_p = 1.2$, the hydrodynamic forces are not strong enough to lift the particle from the bottom wall, as shown in the figure 6 on the left column.

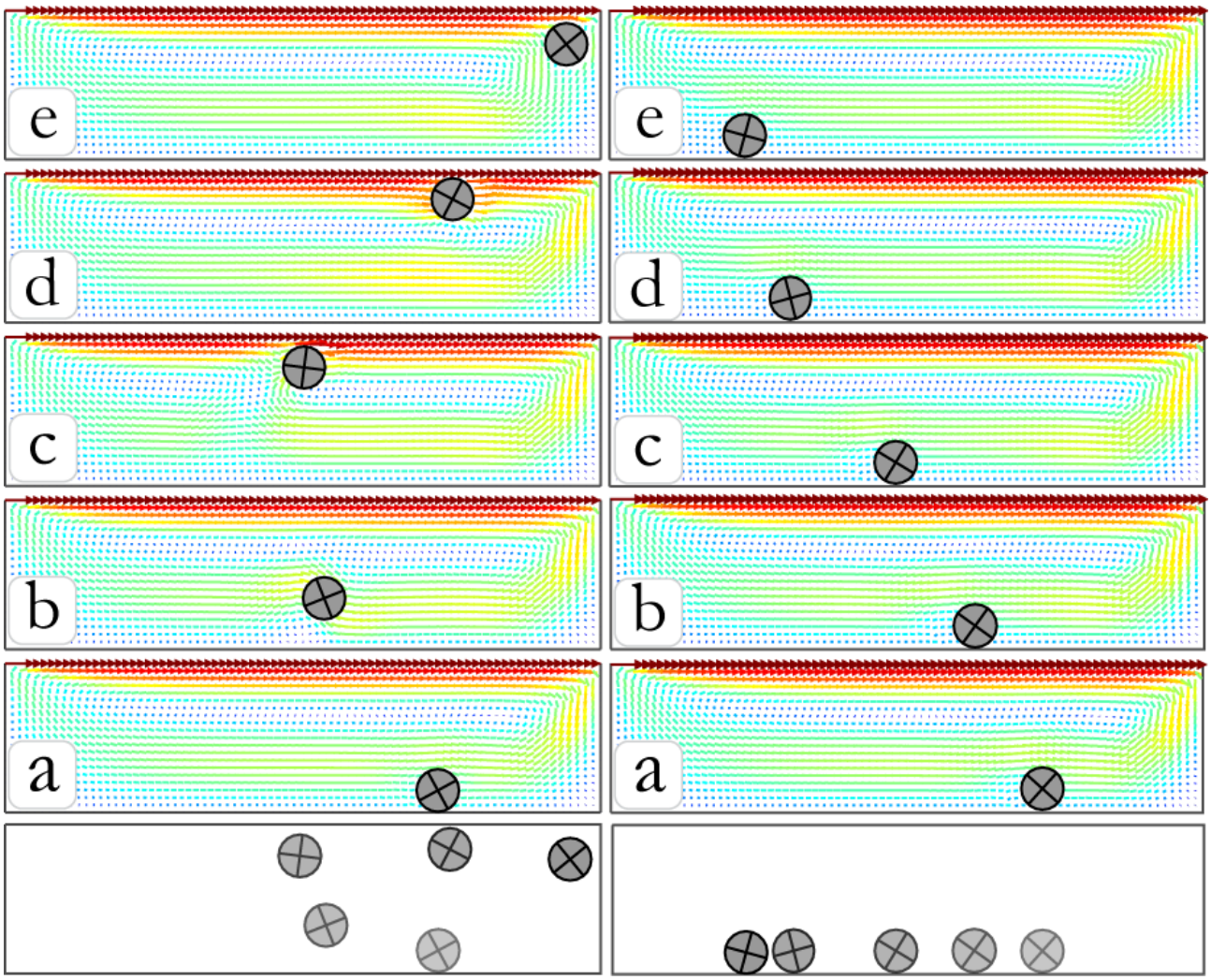

Figure 6. Single particle dragged by the fluid: On the left column we can see the dynamics of a particle lighter than the fluid and on the right column the movement of a particle with density bigger than the fluid's density. The light particle moves upward while the heavy remains at the bottom of the box.

5 CONCLUSIONS

In this work we proposed a new fully implicit–fully coupled finite element formulation for the direct numerical simulation of incompressible fluid flows with suspended rigid particles based on the Lagrange multipliers/fictitious domain method. The solver uses an implicit approach for time discretization and Newton's method for efficiently solve the fully coupled non–linear system of equations obtained at each time step. We recall that all previous works on this research area developed confusing and extensive explicit projection methods to perform numerical solution of the particulate flow problems.

Our method was validated using different test problems that simulate the sedimentation of one or more cylindrical particles in a two-dimensional box. The results obtained were compared with previous numerical and theoretical results and we showed that they have an excellent agreement with the literature.

We are planning to extend this work to perform 3–dimensional simulations and we have already started its adaptation for real life applications such as sedimentation problems to the manufacturing of ordered monolayer of micro and nano particles or sediments transport for example. The technique seems to be very promising tool to study these physical phenomena using direct numerical simulation.

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