Flows with suspended and floating particles

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Abstract

The evolution of the configuration of a set of particles dispersed in a flowing liquid is crucial in many applications such as sedimentation, slurry transport, rheology and structured arrays of micro and nano particles. Direct Simulation based on what is called Fictitious Domain Method coupled with Finite Element Method has been used to study particulate flows and sedimentation process. Here we extend the previously proposed formulations to naturally include buoyancy force and the capillary driven attraction or repulsion of particles located at fluid interfaces. The set of differential equations is discretized using a fully implicit–fully coupled Fictitious Domain/Finite Element approach, avoiding numerical instabilities that may arise from explicit integration. The proposed formulation and implementation are validated by comparing the predictions of simple 2D flows to available numerical or analytical solutions. The method is then used to analyze the flotation of 2D particles and capillary driven aggregation at fluid interfaces.

Keywords: Fluid Simulation, Capillarity Force, Finite Element Method, Fictitious Domain, Lagrange Multipliers

1. Introduction

Flows with suspended particles occurs in many applications such as sedimentation, slurry transport, rheology and formation of structured arrays 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 these processes. In the situations at which particles reach fluid interfaces, capillary forces that may drive particle aggregation and cluster formation need to be included in the analysis.

Different computational techniques have been developed over the years to model flows with suspended particles. The first class of methods computes the velocity and pressure fields of the fluid flow around each individual particle by numerically solving the Navier–Stokes system. The hydrodynamic forces acting on each particle is calculated from the fluid flow solution and is used in the equation that describes the particle motion. In the works of Hu (1996) and Hu et al. (1992), the velocity and pressure fields of the fluid flow were obtained by the finite element method. The finite element mesh had nodes over the fluid–solid boundaries, and those nodes moved with the particle. Therefore, a new mesh needed to be computed at each time step, making this class of methods extremely expensive.

A second class of methods is based on what is called the Fictitious Domain Method. The pioneering work was proposed by Glowinski et al. (1999) and later followed by Diaz-Goano et al. (2001, 2003); Patankar et al. (2000); Veeramani et al. (2005) and Veeramani et al. (2007). In this class of methods, the whole domain, which includes the regions occupied by the fluid and particles, is discretized by a single mesh and an augmented Navier–Stokes equation is solved over the entire domain. Using the Lagrange multipliers technique, the velocity field inside the particles is constrained to a rigid body motion. This approach avoids the need for remeshing at each time step. Typically, the transient response is solved explicitly and an iterative procedure is used to solve the velocity and the pressure field separately.

The description of flows with solid particles at interfaces also follows two different approaches. Singh and Joseph (2005) developed a method that combined level set and Lagrange multipliers to study the evolution of particles at interfaces assuming that the particles were initially at rest along the interface. An alternative approach was used by Fujita and Yamaguchi (2006) to study drying of colloidal particle suspension. Instead of solving the Navier–Stokes equations to compute the forces between the fluid and the particles explicitly, they describe the motion of the particles using Langevin equations, in which forces exerted on each particle consist of contact force, capillarity force, Brownian force, van der Walls force, electrostatic force and fluid drag force, evaluated in the limit of creeping flow, when the Reynolds number is approximately zero.
In this work, we study the flow of liquids with suspended particles that may move towards and float on an interface between immiscible fluids using the fictitious domain approach based on Lagrange Multipliers. Once the particles are located at the interface, capillary forces may cause aggregation of the particles, leading to cluster formation. The resulting differential equations are solved using a fully implicit–fully coupled finite element formulation, which avoids explicit projection methods and time–split integration schemes.

2. Mathematical formulation

In this section we present the governing equations for Newtonian incompressible fluids, the equation of motion of rigid bodies, and capillarity force that acts on particles floating at the interface of two immiscible fluid phases.

2.1. Notation

Consider a two–dimensional bounded domain $\Omega$ with external boundary $\partial \Omega$, which is filled with Newtonian incompressible fluids and suspended solid particles. Whenever the context is clear, we call fluid one or more immiscible, Newtonian and incompressible fluid phases filling the simulation domain $\Omega$.

Figure 1: Sketch of a simulation scenario: two immiscible fluid phases $\Omega_f^1$ and $\Omega_f^2$ filling a two–dimensional box $\Omega$ and one suspended particle covering the region $\Omega_p^i$.

We denote $\Omega_f = \bigcup_{f_i=1}^{n_f} \Omega_f^i$ the region of $\Omega$ occupied by $n_f$ fluid phases $f_i \in \{1 \ldots n_f\}$ with densities $\rho_{f_i}$ and viscosities $\mu_{f_i}$, and we denote $\Omega_p = \bigcup_{p_i=1}^{n_p} \Omega_p^i$ the region of $\Omega$ covered by $n_p$ rigid particles $p_i \in \{1 \ldots n_p\}$ with densities $\rho_{p_i}$ and radius $R_{p_i}$. We also represent the interface between fluid
and particles by \( \partial \Omega_p = \bigcup_{i=1}^{n_p} \partial \Omega_{p_i} \), where \( \partial \Omega_{p_i} \) represents the boundary of the particle \( p_i \) and we denote the interface between two fluid phases \( f_i \) and \( f_j \) by \( \partial \Omega_{f_i f_j} \). Finally, we observe that \( \Omega = \Omega_f \bigcup \Omega_p \). Figure 1 sketches a typical simulation scenario with a two dimensional domain filled by two fluid phases and one suspended solid particle.

### 2.2. Governing equations

The fluid motion is described by the momentum and mass conservation equations:

\[
\rho_{f_i} \frac{D \vec{u}_{f_i}}{Dt} = \nabla \cdot \sigma_{f_i} + \vec{g} \quad \text{in } \Omega_{f_i} \tag{1}
\]

\[
\nabla \cdot \vec{u}_{f_i} = 0 \quad \text{in } \Omega_{f_i} \tag{2}
\]

where \( \vec{g} \) is the gravity acceleration, \( \vec{u}_{f_i} \) is the velocity and \( \sigma_{f_i} \) is the stress tensor of phase \( f_i \). For Newtonian fluids, the later is:

\[
\sigma_{f_i} = -p_{f_i} \delta + \mu_{f_i} (\nabla \vec{u}_{f_i} + \nabla \vec{u}_{f_i}^T) \tag{3}
\]

where \( p_{f_i} \) is the pressure and \( \delta \) the identity tensor.

Let us denote the velocity of the centroid \( \vec{X}_{p_i} \) of a particle \( p_i \) by \( \vec{U}_{p_i} \) and its angular velocity by \( \omega_{p_i} \). The rigid body motion equations for a rigid particle are written as:

\[
M_{p_i} \frac{\partial \vec{U}_{p_i}}{\partial t} = M_{p_i} \vec{g} + \vec{H}_{p_i} \quad \text{in } \Omega_{p_i} \tag{4}
\]

\[
I_{p_i} \frac{\partial \omega_{p_i}}{\partial t} + \omega_{p_i} \times I_{p_i} \omega_{p_i} = \vec{T}_{p_i} \quad \text{in } \Omega_{p_i} \tag{5}
\]

where \( M_{p_i} \) is the mass of the particle, \( \vec{H}_{p_i} \) is the hydrodynamic plus any other body force acting on the particle, \( I_{p_i} \) is its inertial tensor and \( \vec{T}_{p_i} \) is the hydrodynamic plus any other body torque about its center of mass.

### 2.3. Capillarity force

It is frequently observed that particles floating on a liquid interface are subjected to forces which in most cases tend to produce clusters of particles. The particles may be either attracted to a wall or to each other to form such clusters. The attraction (or repulsion) force between particles is a direct consequence of the interface deformation caused by nearby particles, that leads to a non symmetric configuration of the contact line and interface, as sketched in figure 2. In case of hydrophilic particles (2 a), a convex meniscus
Figure 2: Configuration of the interface between two fluids, deformed due to the presence of two particles located near each other. (a) Lower fluid wets the particles, (b) upper fluid wets the particles.

is formed and the interface is higher in the small space between the particles. In the case of hydrophobic particles (2 b), a concave meniscus is formed and the interface height is lower between the particles. As discussed by Gifford and Scriven (1971), the resultant capillary attraction force is a combination of two different contributions. As sketched in figure 3, the horizontal component of the interfacial tension force that acts along the contact line is stronger in the side facing the nearby particle. The second contribution is related to the pressure difference acting on the particle surface. The higher contact line position in the side facing the other particle creates a sub ambient pressure smaller than the atmospheric pressure on the other side.

Gifford and Scriven (1971) evaluated the effective horizontal force per unit length of a horizontal cylinder floating in the interface between two fluids which would have to be applied to keep the cylinders from moving towards each other, i.e. at an equilibrium state. This force represents the horizontal component of the net effect of the capillary action related to the interface deformation near floating particles. It is a function of the wetting characteristics of the particle (contact angle), the interfacial tension between the fluids, the fluid densities $\rho_{f_1}$ and $\rho_{f_2}$ and particle size $R_{p_i}$ and density $\rho_{p_i}$. Similar approach has been used by Kralchevsky and Nagayama (2000) to compute the lateral force acting on spherical particles separated by certain distance. They show, as for horizontal cylinders, that the attractive (or repulsive) force decays rapidly as the particles are moved apart. The calculation of Gifford and Scriven (1971) shows that the horizontal net capillary
force acting on a floating horizontal cylinder is given by:

\[ \vec{c}_{h}^{p_{i}} = AR_{p_{i}}^{4} \left( \frac{\rho_{f_{2}} - \rho_{f_{1}}}{\varsigma} \right)^{2} \exp \left\{ -d \sqrt{\frac{g (\rho_{f_{2}} - \rho_{f_{1}})}{\varsigma}} \right\} \vec{i} \]  \hspace{1cm} (6)

where \( R_{p_{i}} \) is the cylinder radius, \( d \) is the distance between two neighboring particles and the constant \( A \) is a function of the wetting properties.

The attractive force virtually vanishes if the particles are at a distance larger that \( d \approx 5 \sqrt{\frac{\varsigma}{g (\rho_{f_{2}} - \rho_{f_{1}})}} \) apart from each other.

The vertical component of the capillary force is a result of the interfacial tension force acting along the contact line. It is a function of the interfacial tension \( \varsigma \), contact angle \( \psi \) and the contact line position on the particle surface, defined by \( \theta_{1} \) and \( \theta_{2} \) (see figure 3):

\[ \vec{c}_{v}^{p_{i}} = \varsigma \left[ \sin(\psi + \theta_{1} - \pi) + \sin(\psi + \theta_{2} - \pi) \right] \]  \hspace{1cm} (7)

In our formulation, presented in the following section, we describe the capillary action in each particle that intersects the interface between two fluids as an external body force. The horizontal and vertical components of this force are based on equations 6 and 7 respectively. The approach of representing the net capillary force as body force has been used successfully by Fujita and Yamaguchi (2006). The great advantage of this approach is that a detailed description of the interface near the particles can be avoided, eliminating the need of extremely fines meshes and expensive computations.
3. Numerical approximation

In this section we describe a new formulation for modeling flows of liquids with suspended and floating particles using the well–known technique called fictitious domain introduced by Hyman (1952). The formulation presented here is a variation of that presented by Diaz-Goano et al. (2003), including not only the effects of the capillarity forces acting on particles at fluid interfaces but also the computation of the buoyancy force as the integral over the particle surface of the normal component of the liquid traction.

3.1. Fictitious domain

Fictitious domain methods comprise a large class of solution methods for partial differential equations. The basic idea is to extend a problem defined on a geometrically complex and possibly time–dependent domain to a larger and simpler one called the fictitious domain (see figure 4). This conceptual framework provides two key advantages in constructing computational schemes:

– The extended domain is geometrically simpler, so it admits more regular meshes which makes it easier to design efficient codes for solving the partial differential equations.

– The extended domain may be time–independent even if the original domain is time dependent, thus the same fixed mesh can be used for the entire computation, eliminating the need of remeshing algorithms.

The boundary conditions of the original problem must still be enforced, in order to the solution of the extended problem to match the solution on the original domain. Simulations of flows with suspended particles based on the fictitious domain method (see the works of Glowinski et al. (1999); Diaz-Goano et al. (2003)) choose the region occupied by the fluid to be the original complex domain, and the extended domain to be the region occupied by the fluid together with the particles. The no–slip condition along the particles’ boundary is enforced as a side constraint, using a Lagrange multipliers field over the particles region.
3.2. Flows with suspended particles

To begin the derivation of the differential formulation of the problem using the fictitious domain method, let us define the velocity field $\vec{u}_p$ to be a rigid body velocity inside each particle $p_i$ and zero in the fluid region $\Omega_f$, i.e.:

$$\vec{u}_p = \begin{cases} \vec{U}_p + \omega_p \times (\vec{x} - \vec{X}_p) & \text{in } \Omega_p_i \text{ with } p_i \in (1 \ldots n) \\ 0 & \text{in } \Omega_f \end{cases} \quad (8)$$

The integral momentum equation for $\vec{u}_p$ restricted to $\Omega_p_i$ can be written as follows:

$$\int_{\Omega_p_i} \rho_{p_i} \frac{D\vec{u}_p}{Dt} \, d\Omega_{p_i} = \int_{\Omega_p_i} \rho_{p_i} \vec{g} \, d\Omega_{p_i} + \int_{\partial\Omega_{p_i}} \vec{n}_{p_i} \cdot \sigma_f \, d\partial\Omega_{p_i} + \vec{b} \quad (9)$$

where $\vec{n}_{p_i}$ is the outward normal to $\partial\Omega_{p_i}$ and $\vec{b}$ represents the capillary, repulsion or any other body force acting on the particle.

It is important to notice that the surface integral term on the previous equation includes the total hydrodynamic force and torque acting on the surface of particle $p_i$. Diaz-Goano et al. (2003) derived their formulation for flows with suspended particles starting from an expression quite similar to Equation 9. The main difference between our approach and Diaz-Goano’s formulation is that the particle’s weight, the second integral term on the previous equation, is written by Diaz-Goano et al. as the particle’s relative
weight with respect to the liquid. In our approach, we used the absolute particle’s weight instead, since the buoyancy force will appear naturally as a result of integral of the liquid pressure field over the particle boundary. Our approach is conceptually appropriate to perform simulations in which the particle is suspended in more than one fluid phase, since the buoyancy force action is computed according to the properties of each fluid phase and the position of the particle relative to the liquid–liquid interface.

To simplify the notation, from now on, we will call \( \vec{u}_f \) and \( p_f \) the velocity and pressure fields of all fluid phases. Assuming that the liquid is Newtonian, the stress tensor \( \sigma_f \) can be extended over the entire domain \( \Omega \). Such extension can always be done if we define \( \vec{u} \) and \( p \) to be extensions over \( \Omega \) of the velocity and pressure fields \( \vec{u}_f \) and \( p_f \) of the fluid phase satisfying \( \vec{u} \mid_{\Omega_f} = \vec{u}_f \) and \( p \mid_{\Omega_f} = p_f \). The extended stress tensor, denoted by \( \sigma \), is given by:

\[
\sigma = -p \delta + \mu (\nabla \vec{u} + \nabla \vec{u}^t)
\] (10)

Using this extended stress tensor we can apply the divergence theorem and rewrite equation 9 as:

\[
\int_{\Omega_{p_i}} \rho_{p_i} \frac{D\vec{u}_{p_i}}{Dt} d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i} \vec{g} d\Omega_{p_i} + \int_{\Omega_{p_i}} \nabla \cdot \sigma d\Omega_{p_i} + \vec{b}.
\] (11)

Now, if we adopt the following notation:

\[
\vec{F} = \begin{cases} 
-\rho_f \frac{D\vec{u}}{Dt} + \mu \Delta \vec{u} & \text{in } \Omega_{p_i} \text{ with } p_i \in (1 \ldots n) \\
0 & \text{in } \Omega_f
\end{cases}
\] (12)

together with an additional constraint to the extended velocity field \( \vec{u} \) that imposes \( \vec{u} = \vec{u}_p \) in \( \Omega_p \), the momentum equation for particle \( p_i \) becomes:

\[
\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{D\vec{u}_{p_i}}{Dt} d\Omega_{p_i} = \int_{\Omega_{p_i}} \left\{ \rho_{p_i} \vec{g} - \nabla p + \vec{F} \right\} d\Omega_{p_i} + \vec{b}.
\] (13)

We can interpret the additional force per unit of volume \( \vec{F} \) in the previous equation as the force that avoids deformations inside the particle’s region and also enforces the buoyancy force action on the particles. It is important to note that our formulation is different from Diaz-Goano et al. (2003) approach. In their formulation, the additional force \( \vec{F} \) was chosen in order to vanish.
the stress tensor $\sigma$ inside the region filled by particles, which removes the hydrodynamic forces and torque terms from the equations.

Since $\vec{u}$ describes a rigid body motion inside each particle $p_i$, $\vec{u} = \vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})$ in $\Omega_{p_i}$, and the region $\Omega_{p_i}$ is invariant with respect to time, i.e. the particle’s shape is fixed (circular in this work), we can write the equation for the particle’s velocity $\vec{U}_{p_i}$ from equation 13 as:

$$\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{\partial \vec{U}_{p_i}}{\partial t} \, d\Omega_{p_i} = \int_{\Omega_{p_i}} \left\{ \rho_{p_i} \vec{g} - \nabla p + \vec{F} \right\} \, d\Omega_{p_i} + \vec{b}.$$  \hspace{1cm} (14)

We can recover the angular velocity $\omega_{p_i}$ assuming the no-slip boundary condition along the surface of particle $p_i$, $\vec{u} = \vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})$ in $\partial \Omega_{p_i}$. From this assumption, using Stokes’ theorem and properties of the curl operator, we can write the following equation for the particle’s angular velocity:

$$\int_{\Omega_{p_i}} \omega_{p_i} \, d\Omega_{p_i} = \frac{1}{2} \int_{\Omega_{p_i}} \nabla \times (\vec{u} - \vec{U}_{p_i}) \, d\Omega_{p_i}.$$ \hspace{1cm} (15)

Using the definition of the fictitious force $\vec{F}$, the extended velocity $\vec{u}$, pressure $p$ and stress tensor $\sigma$ fields, we can rewrite the momentum equation 1 for the fluid phase:

$$\rho \frac{D\vec{u}}{Dt} = \nabla \cdot \sigma + \vec{g} - \vec{F} \quad \text{in } \Omega.$$ \hspace{1cm} (16)

As we have discussed before, it is clear from equations 14 and 16 that $\vec{F}$ is a term that avoids deformation of the field $\vec{u}$ inside each particle $p_i$. Moreover, the gravity force $\vec{g}$ is considered in the final version of momentum equation 16. The gravity term enforces a hydrostatic pressure in the fluid domain, which is necessary in the analysis of flows with free surfaces or interfaces between immiscible liquids and to get the buoyancy effect naturally from the integration of the pressure force along the particle boundary.

Following Diaz-Goano et al. (2003), we can define a global Lagrange multiplier $\vec{l}$ that is related to $\vec{F}$ through the following boundary value problem:

$$\vec{F} = -\alpha \vec{l} + \mu \triangle \vec{l} \quad \text{in } \Omega$$ \hspace{1cm} (17)

$$\vec{l} = 0 \quad \text{on } \partial \Omega$$ \hspace{1cm} (18)

10
where $\alpha$ is a positive constant parameter.

The problem defined by equations 17 and 18 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 $\vec{l}$ has the same smoothness properties and spatial regularity of $\vec{u}$. The Lagrange multipliers field is non-zero only inside the particles domain, so we can explicitly require $\vec{l}$ to be zero on the fluid region, that is $\vec{l} = 0$ in $\Omega_f$.

In conclusion, the complete formulation of the flow with suspended particles using the fictitious domain method is:

$$
\rho \frac{D\vec{u}}{Dt} = \nabla \cdot \vec{\sigma} + \vec{g} + \alpha \vec{l} - \mu \Delta \vec{l} \\

\nabla \cdot \vec{u} = 0
$$

in $\Omega$

$$
\int_{\Omega_{pi}} (\rho_{pi} - \rho_f) \frac{\partial \vec{U}_{pi}}{\partial t} d\Omega_{pi} = \int_{\Omega_{pi}} \left\{ \rho_{pi} \vec{g} - \nabla p - \alpha \vec{l} + \mu \Delta \vec{l} \right\} d\Omega_{pi} + \vec{b} \\

\int_{\Omega_{pi}} \omega_{pi} d\Omega_{pi} = \frac{1}{2} \int_{\Omega_{pi}} \nabla \times (\vec{u} - \vec{U}_{pi}) d\Omega_{pi}
$$

in $\Omega_{pi}$

(19)

In addition to the system of equations 19, the Lagrange multiplier in the fluid domain, the rigid body constraint inside the particle domain and the evolution of the particles’ position must also be in the complete formulation:

$$
\vec{l} = 0 \\

\vec{u} = \vec{U}_{pi} + \omega_{pi} \times (\vec{x} - \vec{X}_{pi}) \\

\frac{\partial \vec{X}_{pi}}{\partial t} = \vec{U}_{pi}
$$

for $p_i \in (1 \ldots n_p)$

(20)

3.3. Capillary and repulsion forces

As previously stated, the formulation proposed naturally computes the buoyancy forces in each particle and therefore is more adequate to complex flows with particles that float in the interface between two immiscible fluids.

To perform the simulation of floating particles we need also to include the effect of the capillarity forces, described in section 2. The capillarity force,
which appears as a result of the interface deformation near the particles, is treated as a body force acting on the particles that are on the interface between the fluid phases. We adopt the following notation:

\[
\vec{C}_{p_i} = \begin{cases} 
\vec{c}_{p_i} & \text{if } p_i \text{ intersects } \partial \Omega_{f_{ij}} \\
0 & \text{otherwise}
\end{cases}
\] (21)

Equation 21 states that the action of the capillarity force is restricted to particles that intersect the interface \(\partial \Omega_{f_{ij}}\) between two fluid phases \(f_i\) and \(f_j\). Because the capillary force is treated as a body force, there is no need to track the interfacial deformation: in the model proposed here, the interface position is fixed. The advantage of such approach is the reduced computational effort, there is no need to track or capture the interface position nor fine meshes near the interface. The limitation is that the effect of the interface deformation on each individual particle is simplified: it is derived based on net equilibrium capillary forces and the contact line position in each particle located at the interface is not a function of the dynamics of the system nor the contact angle.

Based on the works of Gifford and Scriven (1971) we chose the critical distance beyond which the horizontal interaction force vanishes to be five times the capillary length \(L_c = 5\sqrt{\frac{\varsigma}{g(\rho_f - \rho_l)}}\). Therefore, the horizontal capillary force acting on a particle that intersects the interface is:

\[
\vec{c}_{h_{p_i}} = \begin{cases} 
0 & \text{if } d_{ij} > \delta_c = 5L_c \\
ARp_i^4 \frac{(\rho_f - \rho_l)}{\varsigma} \exp \left\{ -\frac{d_{ij}}{L_c} \right\} & \text{otherwise}
\end{cases}
\] (22)

where \(d_{ij} = \| \vec{X}_{p_i} - \vec{X}_{p_j} \| \) is the distance between the particles’ centers.

The vertical component of the capillary force is related to the surface tension force acting along the contact line. We adopted the expression derived by Gifford and Scriven (1971), equation 7, considering as an approximation \(\theta = \theta_1 = \theta_2 = \ldots = \arccos \left( \frac{h}{R} \right)\), as indicated in figure 3. Therefore:

\[
\vec{c}_{v_{p_i}} = 2\varsigma \sin(\psi + \theta - \pi)
\] (23)

To avoid one particle penetrating another particle or a domain wall, we need to include a repulsion force \(\vec{R}_{p_i}\) on the particle dynamics as proposed by Glowinski et al. (1999). Using particles to represent the walls, we can uniformly treat the repulsion force between a particle \(p_i\) and a particle/wall
The repulsion force only acts if the particles are close enough to each other, i.e. at a distance \( d < \delta_r \). In this work we arbitrarily set \( \delta_r = 0.5R_{pi} \). It rises rapidly as the distance \( d_{ij} \) between particles falls. We computed the repulsion force, as proposed by Glowinski et al. (1999) as:

\[
\vec{R}_{pi} = \sum_{d_{ij} < \delta_r} \beta W(d_{ij})
\]

where \( \beta \) is a “stiffness” parameter that represents a contact force and \( W(d) \) is a weighting function related to the distance between the particles. We considered \( W(d) = \frac{d^2}{4} - d + 1 \), where \( d = \frac{2d_{ij}}{\delta_r} \).

The final formulation including the capillarity force \( \vec{C}_{pi} \) and the repulsion force \( \vec{R}_{pi} \) in the particle dynamics becomes:

\[
\rho \frac{D\vec{u}}{Dt} = \nabla \cdot \vec{\sigma} + \vec{g} + \alpha\vec{l} - \mu \Delta\vec{l}
\]

\[ \nabla \cdot \vec{u} = 0 \]

\[
\int_{\Omega_{pi}} (\rho_{pi} - \rho_f) \frac{\partial \vec{U}_{pi}}{\partial t} d\Omega_{pi} = \int_{\Omega_{pi}} \left\{ \rho_{pi} \vec{g} - \nabla p - \alpha\vec{l} + \mu \Delta\vec{l} \right\} d\Omega_{pi} + \vec{C}_{pi} + \vec{R}_{pi} \text{ in } \Omega_{pi}
\]

\[
\int_{\Omega_{pi}} \omega_{pi} d\Omega_{pi} = \frac{1}{2} \int_{\Omega_{pi}} \left\{ \nabla \times (\vec{u} - \vec{U}_{pi}) \right\} d\Omega_{pi}
\]

\[
\vec{l} = 0 \text{ in } \Omega_f
\]

\[
\vec{u} = \vec{U}_{pi} + \omega_{pi} \times (\vec{x} - \vec{X}_{pi}) \text{ in } \Omega_{pi}
\]

\[
\frac{\partial \vec{X}_{pi}}{\partial t} = \vec{U}_{pi}
\]
its variational form we need to choose the solution space for the physical unknowns of the problem. A natural choice for the fluid’s velocity and pressure, the Lagrange multipliers field and the particle’s velocities is:

\[
\mathbb{C} = \{ (\vec{u}, p, \vec{I}, \vec{U}_p, \omega_p) \mid \vec{u} \in \mathbb{V}, p \in \mathbb{P}, \vec{I} \in \mathbb{L}, \vec{U}_p \in \mathbb{R}^2, \omega_p \in \mathbb{R} \}
\tag{25}
\]

where \(p_i \in (1 \ldots n_p)\) and the spaces \(\mathbb{V}, \mathbb{P}\) and \(\mathbb{L}\) are defined as:

\[
\mathbb{V} := \{ \vec{u} \in H^1(\Omega) \mid \vec{u} |_{\partial\Omega} = 0 \}
\]

\[
\mathbb{L} := \{ \vec{l} \in H^1(\Omega) \mid \vec{l} |_{\Omega_f} = 0 \}
\]

\[
\mathbb{P} := \{ p \in H^0(\Omega) \}
\]

and \(H^k(\Omega_f)\) is the Sobolev space:

\[
H^k(\Omega_f) = \{ w \mid w \in L_2(\Omega_f), \frac{\partial^k w}{\partial x} \in L_2(\Omega_f); \ldots; \frac{\partial^k w}{\partial x} \in L_2(\Omega_f) \}
\]

The variational formulation of the problem is the following:

Find \(\vec{u} \in \mathbb{V}, p \in \mathbb{P}, \vec{I} \in \mathbb{L}, \omega_p \in \mathbb{R}\) and \(\vec{U}_p \in \mathbb{R}^2\) such that \(\forall \vec{\phi} \in \mathbb{H}^1(\Omega)\) and \(\forall \chi \in \mathbb{H}^0(\Omega)\):

\[
\int_{\Omega} \left( \rho_f \frac{D\vec{u}}{Dt} - \vec{g} \right) \cdot \vec{\phi} \, d\Omega = \int_{\Omega} \left( \alpha \vec{l} \cdot \vec{\phi} - \sigma : \nabla \vec{\phi} + \mu \nabla \vec{l} : \nabla \vec{\phi} \right) \, d\Omega \quad \text{in } \Omega
\]

\[
\int_{\Omega} (\nabla \cdot \vec{u}) \chi \, d\Omega = 0 \quad \text{in } \Omega
\]

\[
\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{\partial \vec{U}_p}{\partial t} \, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i} \vec{g} - \nabla p - \alpha \vec{l} \, d\Omega_{p_i} + \vec{C}_{p_i} + \vec{R}_{p_i} \quad \text{in } \Omega_{p_i}
\]

\[
\int_{\Omega_{p_i}} \omega_p \, d\Omega_{p_i} = \frac{1}{2} \int_{\Omega_{p_i}} \nabla \times (\vec{u} - \vec{U}_p) \, d\Omega_{p_i} \quad \text{in } \Omega_{p_i}
\]

\tag{26}

Observe that the last two equations in the differential formulation (see Equation 24) are integral and algebraic equations that are used to determine the unknowns \(\vec{U}_p\) and \(\omega_p\) and therefore they must be incorporated into the final variational system. Moreover, we used the divergence theorem on the Laplacian terms to rewrite the fluid’s momentum and the particle’s velocity.
equations. The integrals over the domain’s boundary $\partial \Omega$ (in the fluid’s momentum equation) and over the boundaries of particles $\partial \Omega_{p_i}$ (in the particle’s velocity equation) were removed from the final weak formulation. The first boundary integrals will be enforced as Neumann boundary conditions for the velocity $\vec{u}$ and the Lagrange multipliers $\vec{l}$ fields. The last boundary integral over the particle’s surface will be neglected because, as we will discuss in the next section, the particle’s boundary are not explicitly represented in our approach. However, the error induced by this approximation is small and does not degrade the solution obtained by the method, as discussed by Diaz-Goano et al. (2003).

In addition to the system of equations 26, the rigid body constraint for the fluid’s velocity inside the particle’s domain and the Lagrange multipliers equations must be included in the final variational formulation. We must also solve the differential equation that describes the evolution of the particle position. The variational form of this last set of equations is straightforward:

$$\int_{\Omega_f} \vec{l} \cdot \vec{\phi} \, d\Omega_f = 0 \quad \text{in } \Omega_f$$

$$\int_{\Omega_{p_i}} (\vec{u} - \vec{U}_{p_i}) \cdot \vec{\phi} \, d\Omega_{p_i} = \int_{\Omega_{p_i}} \omega_{p_i} (\vec{x} - \vec{X}_{p_i}) \cdot \vec{\phi} \, d\Omega_{p_i} \quad \text{in } \Omega_{p_i}$$

$$\frac{\partial \vec{X}_{p_i}}{\partial t} = \vec{U}_{p_i} \quad \text{for } p_i \in (1 \ldots n_p)$$

(27)

The momentum and the continuity equations are defined over the whole domain $\Omega$, and that is the reason why the weak formulation can be discretized in space on a single and fixed discretization of $\Omega$, avoiding the need of remeshing around the particles. Observe that we must only solve the rigid body constraint, the particle’s velocity and angular velocity equations inside the region covered by particles.

4. Numerical framework

In the Finite Element Method, the infinite dimensional solution space $C$ is replaced by a finite dimensional subspace $C \subset \mathbb{C}$, of finite dimension. The choice of the finite dimensional space $C$ is essentially the choice of the finite element basis. We used the following:

$$C = \{(\vec{u}, p, \vec{l}, \vec{U}_{p_i}, \omega_{p_i}) | \vec{u} \in V, p \in P, \vec{l} \in L, \vec{U}_{p_i} \in \mathbb{R}^2, \omega_{p_i} \in \mathbb{R} \}$$

(28)
were \( p_i \in (1 \ldots n_p) \) and the spaces \( V, P \) and \( L \) are defined as:

\[
V := \{ \vec{u} \in Q_2(\Lambda) \times Q_2(\Lambda) \mid \vec{u} \mid_{\partial \Lambda} = 0 \}
\]

\[
L := \{ \vec{t} \in Q_2(\Lambda) \times Q_2(\Lambda) \mid \vec{t} \mid_{\Lambda_f} = 0 \}
\]

\[
P := \{ p \in Q_1(\Lambda) \}
\]

where \( Q_2 \) and \( Q_1 \) represents biquadratic and bilinear functions inside each element. We used quadrangular elements to build the mesh \( \Lambda \) that approximates the simulation domain \( \Omega \). It is well known that this choice of basis functions satisfies the Babuska–Brezzi condition.

The finite element discretization of the variational formulation 26 and 27 leads to a non-linear system of time-dependent differential equations. We perform the time integration using the implicit Euler method since, in many cases, the problems arising from incompressible Newtonian flow applications are stiff and the use of an explicit method requires impractically small time steps \( \delta t \) to keep the error in the result bounded.

The resulting set of non-linear algebraic equations at each time step was solved all together by Newton’s method:

\[
\left[ \frac{1}{\Delta t} M(\vec{c}^{k+1}) + J(\vec{c}^{k+1}) \right] \Delta \vec{c} = -\vec{r}(\vec{c}^{k+1}, \vec{c}^k)
\]

\[
\vec{c}^{k+1} = \vec{c}^k + \Delta \vec{c}
\]

The index \( k + 1 \) and \( k \) indicates the current and previous time step. The solution vector is \( \vec{c} \), which contains the finite element coefficients of all fields and the position, velocity and angular velocity of each particle. The iteration is repeated until convergence. Here, \( J \) is the Jacobian Matrix and \( M \) is the mass matrix.

To solve the sparse linear system in each Newton’s iteration we use the \texttt{IML++} library that provides sparse matrix representation together with iterative methods to solve linear systems. For more details about \texttt{IML++} see the work of Dongarra et al. (1994).

We numerically compute the integrals of the weak formulation using the Gaussian quadrature method. However, a special attention is necessary when computing the integrals over the particle’s domain, because the boundaries of \( \Omega_{p_i} \) do not coincide with boundaries of elements as sketched in 5.

At elements that contain the surface of a particle, we can choose to execute one of the two options: the first approach considers only the Gaussian

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Figure 5: Gaussian quadrature: only Gaussian points lying inside the particles \( p_i \) are used to integrate over the domain \( \Omega_{p_i} \).

... points that lies inside the particle \( p_i \) to perform the integration over \( \Omega_{p_i} \); the second option adapts the mesh around the particle, that is, a mesh refinement is done without changes on the original mesh for integration propose only. We used the first approach and the choice was based on the simplicity and on the efficiency of the implementation when compared with the subdivision approach. Despite being less accurate, the results show that this scheme works well and that the error on the integral over the particle domain does not compromise the results. Figure 6 shows the variation of the computed area of a circular particle moving along a finite element uniform mesh of square elements with nine Gaussian points. The computed area of each particle was evaluated by \( \int_{\Omega_{p_i}} 1 d\Omega_{p_i} \) using the approximated approach described above. The ratio of the elements’ area to the actual particle’s area was 0.14 (first column, on left) and 0.05 (second column, on right). The first plot in each column shows the evolution of the computed area of a particle with 0.0176 cm\(^2\). The second plot shows the relative error of the computed particle area. If the relative area of the element to the particle is smaller than 0.05 the relative error on the evaluation of the particle area is kept smaller than 5%.

We implemented the proposed formulation using the C++ programming language, and the results obtained are presented in next two sections. We validate our formulation and implementation in sections 5.1, 5.2 and 6.1 by comparing the results with available numerical or exact solutions in different test problems with one or more particles in a closed box. The agreement was
Excellent. We also performed a parametric study of more complex flows not studied before with suspended particles (section 5.3) and floating particles (section 6.2) test problems.

5. Flows with suspended particles

For all results presented here, we included one figure (that is a composition of images) illustrating the evolution of the particles position. The first image in each figure (except in the last three tests) is the overlap of the particle’s position obtained from some chosen key frames of the simulation. The other images are the full representation of each key frame and include also the velocity field of the fluid phase. The velocity vectors are colored according to its magnitude. In all images, the cross mark inside each particle indicates the angular orientation change of the particles during the simulation.

5.1. Sedimentation of a single particle

The first test presented is the sedimentation of one particle in a closed box. The results are shown in figure 7. The complete set of parameters is the following: the domain \( \Omega \) is a closed box with size \([-0.286, 0.286] \times [-1.0, 1.0] \) cm\(^2\), discretized by a mesh of 504 squared elements with \( Q_2-Q_1 \) finite elements basis functions. The fluid phase \( \Omega_f \) is a Newtonian incompressible
fluid with density $\rho_f = 1000 \frac{kg}{m^3}$ and viscosity $\mu_f = 0.01 Pa.s$. A single particle with radius $R_p = 0.0714 cm$ and density $\rho_p = 1500 \frac{kg}{m^3}$ is embedded on the fluid. The particle is initially at rest at $\vec{X}_p = (0, 0.869)$. The time step is $\delta t = 0.001 s$ and the total time of the simulation is 1 s. Finally, following the suggestion of Diaz-Goano et al. (2003), we set the Lagrange multiplier parameter $\alpha$ to be 150. The particle motion creates a symmetric liquid flow, as expected.

Figure 8 shows the evolution of the particle’s velocity for different particle densities, varying from 1500 to 1800 $\frac{kg}{m^3}$. The particle accelerates until it reaches a terminal velocity. The small amplitude oscillation observed is due to the inaccuracy of the evaluation of the integral over the particle domain. The magnitude $U_t$ of the terminal velocity of a cylinder falling in a box in the limiting case of $Re \rightarrow 0$ can be evaluated based on the drag force acting on the cylinder. Pasquali (2000) used an asymptotic solution and showed...
Figure 8: Evolution of the particle’s velocity in the sedimentation case using different densities for the particle: In figure (a) the particle’s density is $1.5 \frac{g}{cm^3}$, in (b) $\rho_p = 1.6 \frac{g}{cm^3}$, in (c) $\rho_p = 1.7 \frac{g}{cm^3}$ and finally in (d) $\rho_p = 1.8 \frac{g}{cm^3}$.

Figure that the drag force is:

$$F_d = \frac{4\pi \mu_f}{\Delta} \frac{3}{2} U_t, \quad \text{where} \quad \Delta = U_0 - \left(1 + \sum_i W_i \Gamma^i \right) \ln(\Gamma) + \sum_i V_i \Gamma^i. \quad (29)$$

The ratio of the cylinder radius to the box half–width is denoted by $\Gamma = \frac{R_p}{w}$, $U_0 = -0.915689$. The infinite series was truncated at $i=10$. The odd-numbered coefficients $W_i$ and $V_i$ vanish. The even-numbered coefficients are shown in Table 1:

<table>
<thead>
<tr>
<th>$W_i$</th>
<th>0.5</th>
<th>$V_i$</th>
<th>1.26654</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W_4$</td>
<td>0.054648</td>
<td>$V_4$</td>
<td>-0.91804</td>
</tr>
<tr>
<td>$W_6$</td>
<td>-0.264629</td>
<td>$V_6$</td>
<td>1.87710</td>
</tr>
<tr>
<td>$W_8$</td>
<td>0.792986</td>
<td>$V_8$</td>
<td>-4.66549</td>
</tr>
</tbody>
</table>

Table 1: Dimensionless coefficients for the computation of the drag force using the asymptotic solution of the Stokes’ problem.
When the terminal velocity is reached, the drag force $\vec{F}_d$ is equal the relative weight of the particle when it reaches the terminal velocity, $F_d = P - E$, $P$ and $E$ are the weight and buoyancy force, respectively. The theoretical expression for the magnitude $U_t$ of the terminal velocity is:

$$U_t = \frac{2}{3} \frac{(\rho_f - \rho_p) R_p^2 g \Delta}{4\pi \mu_f}$$

(30)

The red horizontal line on each graph of figure 8 represents the theoretical terminal velocity obtained using the previous expression. As we can see, the agreement between the terminal velocities is excellent, except for the largest particle density. The reason is that, in this case, the Reynolds number is high, e.g. $Re \approx 10$, and the hypothesis of Stokes flow used in the derivation of equation 30 is no longer valid.

For the flow around a falling cylindrical particle, the Reynolds number is computed using the magnitude of the terminal velocity, the particle radius and the fluid properties:

$$Re = \frac{2\rho_f U_t R_p}{\mu_f}$$

(31)
Figure 10: Zoom in the Lagrange multipliers effect over the velocity field in the particle sedimentation test. The Lagrange multipliers are non–zero only inside the particle region as we can see in figure (a). It enforces the rigid body constraint inside the particle, as we observe in figure (b).

In order to evaluate the effect of the Reynolds number on the terminal velocity, we plot the dimensionless terminal velocity

\[ u = \frac{\mu f U_t}{(\rho_f - \rho_p) R_p^2 g} \]

as a function of Reynolds number in figure 9. If the Reynolds number is above \( Re \geq 1 \), creeping flow approximation cannot be used.

As shown during the derivation of the formulation, the Lagrange multipliers imposes the rigid body constraint to the fluid’s velocity inside the particle’s region \( \Omega_p \), avoiding viscous deformations inside each particle. Figure 10 shows the Lagrange multiplier field and the constrained velocity field solution obtained at a certain time step for the solution, presented in figure 7. The solution is symmetric along a vertical line passing through the center of the particle, keeping the angular orientation unchanged during the entire simulation. In figure 10, the vectors of the Lagrange multiplier are normalized for better visualization, and their modulus are represented by colors that scale from blue to red. The gray circle shows the boundary of the particle’s domain. It is clear that the velocity field inside the particle corresponds to a rigid body motion, which in this particular case is a constant velocity since the angular velocity is zero.
Figure 11: Single particle sedimentation: a particle not aligned with the vertical line that divides the domain, with density 1500 $\frac{kg}{m^3}$ suspended on an incompressible fluid of viscosity $0.001$ Pa.s and density 1000 $\frac{kg}{m^3}$ falling under the gravity force.

The example shown in figure 11 clearly shows the coupling between the flow and the particle dynamics. The problem is the same as the one presented in figure 7, except from the fact that the fluid’s viscosity is now set to be $\mu_f = 0.001$ Pa.s and the particle’s initial position is not aligned with the vertical symmetry line, more precisely $\vec{X}_p = (0.05, 0.869)$. With the lower fluid viscosity, the particle velocity is higher and so is the Reynolds number of the flow $Re = 70$. A periodic flow motion develops in the wake of the cylinder as the result of the von Karman vortices. The asymmetry of the flow is clear in figure 11(c). In this case, the particle does not fall vertically.

5.2. Drafting, kissing and tumbling

The next test is the sedimentation of two cylindrical particles (see figure 12), which is a benchmark for flows with suspended particles and is known as the drafting, kissing and tumbling problem (Glowinski et al. (1999)).

The complete set of parameters for the simulation is the following: the domain $\Omega$ is a closed box with dimensions $[-0.5, 0.5] \times [-1.0, 1.0]$ cm$^2$, discretized by a mesh of 350 square elements with $Q_2$-$Q_1$ finite elements basis functions. The fluid phase $\Omega_f$ is a Newtonian incompressible fluid with den-
Figure 12: Two particles sedimentation: two particle of density $1.5 \text{ g cm}^{-3}$ suspended on an incompressible fluid of viscosity $0.01 \text{ Pa.s}$ and density $1.0 \text{ g cm}^{-3}$ falling under the gravity force. We can observe the simulation reproduces the particles iteration dynamics usually called drafting, kissing and tumbling.

The density of the fluid $\rho_f = 1000 \text{ kg m}^{-3}$ and viscosity $\mu_f = 0.01 \text{ Pa.s}$. Two cylindrical particles with radius $R_{1,2} = 0.0514 \text{ cm}$ and density $\rho_{1,2} = 1500 \text{ kg m}^{-3}$ are suspended on the fluid. The particles are initially at 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 $\delta t = 0.001 \text{ s}$ and the total simulated time is $1 \text{ s}$. Again, we set the Lagrange multiplier parameter $\alpha$ to be 150, following Diaz-Goano et al. (2003).

Particle pair interaction is key phenomenon in all practical applications of flows with suspended particles. The flow generated by one particle motion contributes to the motion of the other particles.

When one falling cylinder enters the wake of another, it experiences reduced drag, drafts downward toward the leading particle, and almost touches it, a phenomenon generally referred to as kissing. 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 migration.

The drafting, kissing and tumbling dynamics can be easily observed in figures 12 and 13. The blue lines on the plots of figure 13 refers to the particle initially at the higher position, and the red ones describe the position and velocity of the particle initially at the lower height. Again, the small
amplitude velocity oscillation is caused by the approximation on evaluating the integral over the particle domain.

Analyzing the plots, we observe that the *drafting stage* takes place from the beginning of the simulation until approximately 0.25 s, since the vertical distance between the particles falls until the curves cross at 0.25 s. This indicates that the particle initially at the higher position was on the wake of the lower particle, which increased its velocity. The *kissing stage* begins near 0.25 and goes until 0.375 s. Finally, in the *tumbling stage* we observe that the horizontal distance between the particles rises until reaching a steady distance. At this point the horizontal velocity approaches zero and the particles are falling side by side. The total simulation time was 1 s and the particles reach the bottom wall at $t \approx 0.8$ s. The predicted trajectories show the same features of those presented by Glowinski et al. (1999) and Wan and Turek (2007). A quantitative comparison between the trajectories is not possible because the exact initial location of particles is not provided in the literature.
5.3. Particles dragged by the fluid

The next test problem studies the motion of cylindrical particles that are dragged by the flow inside a lid–driven cavity. The aim of this test is to show the capability of the method to study sediment transport.

The lid–driven cavity flow has been used as a validation problem for new codes or new solution methods because the problem geometry is simple, the boundary conditions are also easy to implement numerically and the flow is quite complex with the presence of recirculation. 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 wall (with tangential velocity). In our test case, a solid cylindrical particle is suspended in the fluid.

The complete set of parameters for the simulations shown in figure 14 is...
the following: the domain $\Omega$ is a closed box with dimensions $[-1.0, 1.0] \times [-0.25, 0.25]$ cm$^2$ with a lid that moves with velocity $\vec{u}_l = (0.1, 0)$ m/s. The domain is discretized by a mesh of 400 square elements. The fluid phase $\Omega_f$ is a Newtonian incompressible fluid with density $\rho_f = 1000$ kg/m$^3$ and viscosity $\mu_f = 0.01$ Pa.s. One particle with radius $R_p = 0.0714$ cm is embedded in the fluid.

The particle is initially at rest at position $\vec{X}_p = (0.6, -0.177)$. The sequence shown in the left column of figure 14 presents the results for particle density equals to $1500$ kg/m$^3$; while the right column presents the results for a particle density equals to $500$ kg/m$^3$. The simulation’s time step is $\delta t = 0.002$ s and the total time $1$ s. The Lagrange multiplier parameter is $\alpha = 150$.

Observe that if the particle’s density is larger than the fluid’s density (see figure 14, left column) the hydrodynamic forces are not strong enough to lift the particle from the bottom wall so it is dragged towards the left with a rolling motion until the end of the simulation. When the particle is lighter than the fluid (see figure 14, right column), it moves upwards and it ends up floating near the up–right corner of the cavity.

The effects of the flow operating conditions on the particle trajectory inside the cavity is illustrated in figure 15. The left column of the figure presents the evolution on the vertical and horizontal positions of the particle for $\rho_p = 320, 500, 1000$ and $1500$ kg/m$^3$. The lift force is weak enough such that only particles lighter than the liquid ($\rho_p = 320, 500$) are suspended.
The effect of the lid velocity at a constant particle density \((\rho_p = 1000)\) is shown in the middle column of figure 15. At low velocity, the vertical hydrodynamic force is weak and particle remains at the bottom of the cavity \((y \approx -0.177)\). As the lid velocity rises, the hydrodynamic force acting on the particle increases, lifting the particle from the bottom of the cavity. The right column of figure 15 shows the effect of the cavity width on the particle trajectories. As the width falls, the pressure gradient across the cavity rises leading higher liquid velocity. Consequently, the particle inside the narrow cavity rises before the other ones.

6. Flows with suspended and floating particles

6.1. Single particle flotation

In this section we validate the floating particles formulation, observing the dynamics and the equilibrium position of a particle as it moves towards the interface between to fluids with different densities, one heavier and one lighter than the particle. Whenever possible, we compare the results to those obtained by Singh and Joseph (2005) that computed the interface position and capillarity force and did not modeled it as a body force. The comparison is only qualitative because their results are for a sphere floating on an interface and ours are for a horizontal cylinder. The basic setup in the next examples is the following: the domain \(\Omega\) is a closed box with dimensions \([-1.1, 1.1] \times [-0.5, 0.5]\) cm\(^2\) discretized by a mesh of 254 square elements and filled with two Newtonian incompressible fluid phases \(\Omega_{f1}\) and \(\Omega_{f2}\). The density and the viscosity of the upper and lower fluid phases are different in each example and will be defined latter for each test case. One particle with radius \(R_p = 0.14\) cm is suspended in the fluid and is initially at rest at the position \((0.0, -0.25)\).

Figure 16 shows the evolution and the final position obtained at three different particle densities. In this case the density of each fluid phase was \(\rho_{f1} = 1000\) kg m\(^{-3}\) and \(\rho_{f2} = 0.0\) kg m\(^{-3}\) and their viscosity \(\mu_{f1} = 0.01\) Pa.s and \(\mu_{f2} = 0.001\) Pa.s. From left to right in figure 16, the particle’s density \(\rho_p\) was 300, 500 and 800 kg m\(^{-3}\). The interfacial tension was not considered in this example. The goal was to check if the formulation and its implementation would give the correct equilibrium position based on the balance between the particle weight and buoyancy force.

In the equilibrium position, the immersed volume \(V_s\) must be equal to \(V_s = \frac{\rho_p}{\rho_{f1}} V_p\). So, for \(\rho_p = 300, 500\) and 800 kg m\(^{-3}\), the theoretical immersed
Figure 16: Single particle sedimentation: the equilibrium height of flotation varies when we change the particle’s density. From left to right, its value was set to be $\rho_p = 300 \text{ kg m}^{-3}$, $\rho_p = 500 \text{ kg m}^{-3}$ and $\rho_p = 800 \text{ kg m}^{-3}$. Volumes $V_s$ must be 0.3, 0.5 and 0.8 cm$^3$. In our code, the immersed volumes obtained were 0.3117, 0.4864 and 0.8189 cm$^3$ that represents an error of around 2% and shows that the equilibrium state obtained by our code agrees with the theory.

The vertical component of the velocity for $\rho_p = 500 \text{ kg m}^{-3}$ is shown in figure 17. As discussed in Singh and Joseph (2005), the behavior is that a spring–dashpot–mass system. Our simplified model is able to describe correctly the behavior of the system.

6.2. Capillarity-driven particle aggregation

The last problem is related to the evolution and final arrangement of a set of particles floating at the interface between two fluid phases. As we said
Figure 17: Vertical component of the velocity for a particle with density \( \rho_p = 500 \ \frac{kg}{m^3} \).
The left graph shows the velocity profile when the particle was initially in the lower fluid \((\rho_{f1} = 1000 \ \frac{kg}{m^3})\) and right shows the velocity evolution of the particle initially in the upper fluid \((\rho_{f2} = 100 \ \frac{kg}{m^3})\).

before, one of the physical phenomena that determines this final arrangement of a set of particles is the capillarity force that occurs due to particle–particle and particle–wall interactions. We show that the final arrangement of the particles is a strong function of their initial configuration.

For all examples shown in this section, the basic set of parameters is the following: the domain \( \Omega \) is a closed box with dimensions \([-1.0, 1.0] \times [-0.5, 0.5] \ \text{cm}^2 \), discretized by a mesh of 253 square elements with \( Q_2-Q_1 \) finite elements basis functions. The fluid phase \( \Omega_f \) is filled with two Newtonian incompressible fluid phases with interface height at \( y = 0.7 \ \text{cm} \). The lower phase’s density is \( \rho_{f1} = 1000 \ \frac{kg}{m^3} \) and its viscosity is \( \mu_{f1} = 0.01 \ \text{Pa.s} \). The upper fluid parameters are set to \( \rho_{f2} = 0.0 \ \frac{g}{cm^3} \) and \( \mu_{f2} = 0.01 \ \text{Pa.s} \). Particles with radius \( R_p = 0.14 \ \text{cm} \) are suspended on the fluid. The particles are initially at rest in random positions. The simulation’s time step is \( \delta t = 0.001 \ \text{s} \) and the total simulated time is 1 \( \text{s} \). We set the Lagrange parameter \( \alpha \) to be 150.

Figure 19 shows the evolution of two particles for two different initial positions. In the left column, the particles were initially located at \( \vec{X}_{p1} = [-0.5, -0.15] \) and \( \vec{X}_{p2} = [0.5, -0.15] \). In the right column, the particles were initially located at \( \vec{X}_{p1} = [-0.25, -0.15] \) and \( \vec{X}_{p2} = [0.25, -0.15] \). Because the particles have lower density than the bottom liquid, they move upward until reaching the interface between the two liquid phases. For the second initial condition (right column), the distance between the two particles once they reach the interface is less than the critical condition \( d < 5L_c \), such that capillary force brings the particles together. Particle aggregation does not
Figure 18: At left, we show the evolution of the centers distance (in units of particle radius) and at right the attraction speed between two particles floating at the two liquid interface.

occur in the results presented in the left column of figure 19: the distance between the particles at the interface is larger than the capillary attraction range.

The evolution of the distance (in units of particle radius) between particles center and the attraction speed is shown in figure 18. The attraction speed first rises until reaching a maximum. After that point, the liquid pressure between the particles need to become strong enough to drive the liquid away and starts to slow down the attraction. These results show the same behavior reported by Singh and Joseph (2005) using a complete level set/fictitious domain approach. As discussed before, this approach is more accurate, but also more computationally expensive. Our approach is approximated and less expensive, but it was able to reproduce the same behavior.

Figure 20 illustrates the motion of five particles initially at rest on the upper (lower density) fluid phase. The particles fall down, drop in the lower fluid phase, float at the interface, forming clusters due to action of the horizontal capillarity force. The left column shows the particles falling and dropping in the lower fluid, while the left column details the clustering process. In this example the original set of particles creates two clusters one with four particles that are attracted to the left wall and the other with one particle attracted to the right wall. This example shows the potential of our method to a further study of the clustering formation problem, given a large number of particles.

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Figure 19: Two particles floating at the fluids interface: the particles are not near enough in the left column so the horizontal component of capillarity force doesn’t exist and the particles are not attracted to each other. On the other hand, on the right column when the particles are close enough when they reach the interface they are attracted to each other.
Figure 20: Floating particles clustering: five particles initially at rest on the upper fluid phase that are falling down, drop in the lower fluid phase (left column) and after floating at the two fluids interface, form two clusters near the walls due to action of the horizontal capillarity force (right column).
7. Final remarks

We proposed a new formulation for the direct numerical simulation of one or more Newtonian incompressible and immiscible fluid phases with suspended and floating rigid particles based on the fictitious domain method using Lagrange multipliers. The buoyancy force acting on each particle appears naturally as a resultant of the integral of the pressure along the particle surface and does not need to be included as an external body force.

The finite element based solver uses an implicit approach for time discretization and Newton’s method for efficiently solving the fully coupled non-linear system of equations obtained at each time step. This avoids the use of explicit projection methods to perform the numerical solution of problems on flows with suspended particles.

We validate the method and implementation using different tests that simulate the sedimentation and the flotation of one or more particles. We compared the results obtained with previous numerical and theoretical results and they showed an excellent agreement in the case of sedimentation. For floating particles, a direct comparison was not possible, since we were able to find only results for spherical particles. Our simplified approach to model capillary interaction was able to describe the correct behavior as predicted by the complete model by Singh and Joseph (2005) for spheres. Moreover, we performed tests in more complex examples that have not been well studied in literature.

This formulation is being extended to perform 3-dimensional simulations with the goal to study the manufacturing of ordered monolayer of micro and nano particles. The technique seems to be a very promising tool to study these physical phenomena using direct numerical simulation.

References


