4
Flows with suspended particles

In this chapter we describe a new formulation for modeling flows with suspended particles using the well–known technique called fictitious domain (23). This new formulation is one of the main contributions of this work. It modifies the formulation of Diaz-Goano et al (2003) (9), adjusting the action of the buoyancy force over the particles and including the gravity force contribution on the fluid's equations. We show that our new formulation is based on a constraint force that avoids viscous deformations and enforces rigid–body motion inside the particles.

This chapter is organized as follows: the first section 4.1 reviews the fictitious domain concept. In Section 4.2 we derive the differential formulation for particulate flows using the fictitious domain method. In Section 4.3 we write the variational version of these equations and finally in Section 4.4 we discuss a fully implicit and coupled method to discretize the variational formulation using the finite element method and an implicit time integrator.

4.1
Fictitious domain methods

Fictitious domain methods comprise a large class of solution methods for partial differential equations and were introduced by Hyman (1952) (23). 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 4.1). 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 and improves their numerical solution stability.
- 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 using remeshing algorithms.

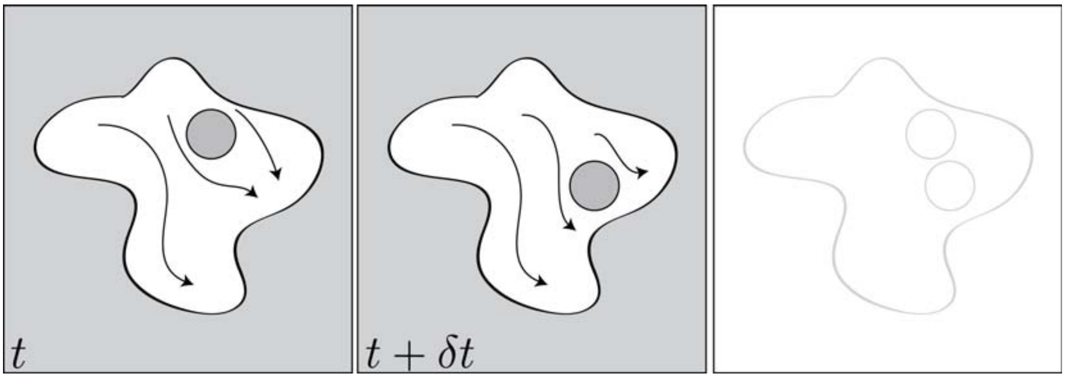

Figure 4.1: Fictitious domain: a problem defined on a geometrically complex domain (white region on the first two pictures), extended to a larger and simpler fictitious domain (white region on the last image).

Of course, the boundary conditions on the original boundary must still be enforced, in order to the solution of the extended problem to match the solution of the original problem on the original domain.

The first works using the fictitious domain technique to simulate fluid–particle interactions were proposed by Glowinski et al. (18, 20). In those papers, the authors described a method to study viscous unsteady flows around rigid particles, which have prescribed motions. Later, Glowinski et al. (19) proposed a more general method that simulates the motion of particles caused by the hydrodynamic forces and torque.

Originally, simulations of flows with suspended particles based on the fictitious domain method 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 interior of the particles. The no–slip condition on the particles' boundary is enforced as a side constraint, using an auxiliary mesh of Lagrange multipliers inside the particles region.

More recently, Diaz-Goano et al. (9) improved Glowinski method, avoiding the need of maintaining auxiliary meshes inside the particles. In this thesis we use Diaz-Goano's methodology, but we modify the formulation in order to correctly account for the fluid–particles interaction forces and to include the gravitational force action on the fluids' governing equations.

4.2 Formulation of flows with suspended particles using fictitious domain

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

$$\vec{u}_p = \begin{cases} \vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i}) & \text{in } \Omega_{p_i} \text{ with } p_i \in (1 \dots n) \\ 0 & \text{in } \Omega_f \end{cases} \tag{4-1}$$

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

$$\int_{\Omega_{p_i}} \rho_{p_i} \frac{\mathrm{D}\vec{u}_p}{\mathrm{Dt}}\, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i} \vec{g}\, d\Omega_{p_i} + \int_{\partial\Omega_{p_i}} \vec{n}_{p_i} \cdot \boldsymbol{\sigma}_f\, d\partial\Omega_{p_i} \tag{4-2}$$

were $\vec{n}_{p_i}$ is the outward normal to $\partial\Omega_{p_i}$.

It is important to notice that the surface integral term on the previous equation includes the total hydrodynamic force and torque acting on particle p_i. Diaz-Goano et al (9) derived their formulation for flows with suspended particles starting from a expression quite similar to Equation 4-2. 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. In our approach, we used the absolute particle's weight instead, since the relative weight represents the absolute particle's weight under the action of the buoyancy force. However, the total hydrodynamic force acting on the particle boundary already includes the buoyancy force. Conceptually, using the relative weight implies that the buoyancy force is being computed twice in the momentum equation for the field $\vec{u}_p$ inside Ω_{p_i}. Diaz-Goano's formulation may lead to wrong velocities for the particles and unphysical behavior in the particle–fluid interaction.

Assuming that the liquid is Newtonian, the stress tensor $\boldsymbol{\sigma}_f$ can be extended over the entire domain Ω. Such extension can always be done if we define $\vec{u}$ and p to be extensions over Ω of the velocity and pressure fields $\vec{u}_f$ and p_f satisfying $\vec{u}\ |_{\Omega_f} = \vec{u}_f$ and $p\ |_{\Omega_f} = p_f$. The extended stress tensor, denoted by $\boldsymbol{\sigma}$, can be written as:

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta} + \mu(\nabla\vec{u} + \nabla\vec{u}^t).$$

Using this extended stress tensor we can apply the divergence theorem and rewrite equation 4-2 as:

$$\int_{\Omega_{p_i}} \rho_{p_i} \frac{\mathrm{D}\vec{u}_p}{\mathrm{Dt}}\, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i} \vec{g}\, d\Omega_{p_i} + \int_{\Omega_{p_i}} \nabla \cdot \boldsymbol{\sigma}\, d\Omega_{p_i}. \tag{4-3}$$

Now, if we adopt the following notation:

$$\vec{F} = \begin{cases} -\rho_f \dfrac{\mathrm{D}\vec{u}}{\mathrm{Dt}} + \mu\triangle\vec{u} & \text{in } \Omega_{p_i} \text{ with } p_i \in (1 \dots n) \\ 0 & \text{in } \Omega_f \end{cases} \tag{4-4}$$

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

$$\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{\mathrm{D}\vec{u}}{\mathrm{Dt}} \, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i}\vec{g} - \nabla p + \vec{F} \, d\Omega_{p_i}. \tag{4-5}$$

It is very important to observe now that we can see the additional force per unit of volume $\vec{F}$ in the previous equation, as the force that avoids viscous deformations on the fluid inside the particle's region and also enforces the buoyancy force action on the particles. Again, we observe that our formulation is different from Diaz-Goano's (9) approach. In their formulation, the additional force $\vec{F}$ was chosen in order to vanish the stress tensor $\boldsymbol{\sigma}$ inside the region filled by particles, which removes the hydrodynamic forces and torque terms from the equations. This is a consequence of the wrong choice of the particle's weight on equation 4-2. As we will show next, this constraint force $\vec{F}$ enforces the rigid body motion onto the fluid velocity field within each of the particles.

From the previous equation 4-5, reminding that $\vec{u}$ describes a rigid body velocity inside each particle p_i, that is $\vec{u} = \vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})$ in Ω_{p_i}, and regarding the material derivative definition, we can write:

$$\frac{\mathrm{D}\vec{u}}{\mathrm{Dt}} = \frac{\mathrm{D}}{\mathrm{Dt}}(\vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})) = \frac{\partial}{\partial t}(\vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})). \tag{4-6}$$

If we substitute the material derivative of the velocity field $\vec{u}$ by the last term of the equality 4-6 the first integral on the equation 4-5 becomes:

$$\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{\partial \vec{U}_{p_i}}{\partial t} \, d\Omega_{p_i} + \int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{\partial}{\partial t}(\omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})) \, d\Omega_{p_i} \text{ in } \Omega_{p_i}. \tag{4-7}$$

Since the area of the particle domain Ω_{p_i} is time independent and observing that the particle p_i is perfectly circular, we can change the order between the time derivative and integration operators in the second term of equation 4-7, which gives us the following identity:

$$\frac{\partial}{\partial t} \int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f)(\omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})) \, d\Omega_{p_i} = 0. \tag{4-8}$$

Using 4-5, 4-7 and 4-8, we get the final equation for the particle's velocity $\vec{U}_{p_i}$:

$$\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f) \frac{\partial \vec{U}_{p_i}}{\partial t} \, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i} \vec{g} - \nabla p + \vec{F} \, d\Omega_{p_i}. \tag{4-9}$$

We can recover the angular velocity ω_{p_i} assuming a no–slip boundary condition on the surface of particle p_i.

$$\omega_{p_i} \times (\vec{x} - \vec{X}_{p_i}) = (\vec{u} - \vec{U}_{p_i}) \ \text{ in } \ \partial\Omega_{p_i}.$$

Then, clearly we can write:

$$\int_{\partial\Omega_{p_i}} (\omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})) \cdot \vec{n}_{p_i} ds = \int_{\partial\Omega_{p_i}} (\vec{u} - \vec{U}_{p_i}) \cdot \vec{n}_{p_i} ds. \tag{4-10}$$

Using Stokes' theorem and properties of the curl operator, we can write the following equation for the particle's angular velocity:

$$\int_{\Omega_{p_i}} \omega_{p_i} \, d\Omega_{p_i} = \frac{1}{2} \int_{\Omega_{p_i}} \nabla \times (\vec{u} - \vec{U}_{p_i}) \, d\Omega_{p_i}. \tag{4-11}$$

Using the fictitious force $\vec{F}$, the extended velocity $\vec{u}$ and pressure p fields and stress tensor $\boldsymbol{\sigma}$, we can rewrite the momentum equation for the fluid phase (equation 2-1) as follows:

$$\rho \frac{\mathrm{D}\vec{u}}{\mathrm{Dt}} = \nabla \cdot \boldsymbol{\sigma} + \vec{g} - \vec{F} \quad \text{in} \quad \Omega. \tag{4-12}$$

As we observed before, it is now clear from equations 4-9 and 4-12 that $\vec{F}$ is a term that avoids viscous deformation onto the field $\vec{u}$ inside each particle p_i. Moreover, the gravity force $\vec{g}$ is present in the final version of momentum equation 4-12, which is intuitively expected for particulate flows problems. In Diaz-Goano's approach the gravity was left out of the momentum equation. The gravity term is conceptually important since it enforces a hydrostatic pressure profile in the fluid domain, which may be desired in the analysis of free surface or immiscible two phase flows with interface (see Figure 4.2).

The force $\vec{F}$ is non–zero only within the domain of the particles Ω_{p_i} however, its impact on the fluid's velocity is over the entire domain, due to equation 4-12. Substituting $\vec{F}$ by its definition 4-4 in equation 4-12, we see that the extra force $\vec{F}$, as we argued before, represents the force necessary to avoid viscous deformations over the particle's domain. The momentum equation inside the particle becomes the buoyancy force definition:

$$\int_{\Omega_{p_i}} \nabla p \, d\Omega_{p_i} = M_f \vec{g} \tag{4-13}$$

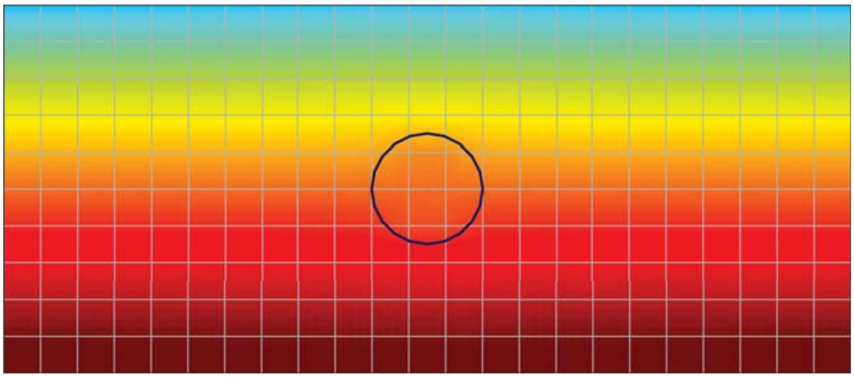

Figure 4.2: Hydrostatic pressure profile obtained by our formulation, using the gravity force on the $\vec{u}$ momentum.

where $M_f = \int_{\Omega_{p_i}} \rho_f \, d\Omega_{p_i}$ represents the fluid mass on region Ω_{p_i}.

Following the approach of Diaz-Goano et al (2003) (9), we can now define a global Lagrange multiplier $\vec{l}$ that is related to $\vec{F}$ through the following boundary value problem:

$$\vec{F} = -\alpha\vec{l} + \mu\triangle\vec{l} \;\text{ in }\; \Omega \tag{4-14}$$

$$\vec{l} = 0 \;\text{ on }\; \partial\Omega \tag{4-15}$$

where α is a positive constant parameter.

The problem defined by equations 4-14, 4-15 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 $\vec{u}$. Observe also that 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 Ω_f.

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

$$\begin{aligned}
&\rho\frac{\mathrm{D}\vec{u}}{\mathrm{Dt}} = \nabla\cdot\boldsymbol{\sigma} + \vec{g} + \alpha\vec{l} - \mu\triangle\vec{l} && \text{in } \Omega\\
&\nabla\cdot\vec{u} = 0 && \text{in } \Omega\\
&\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f)\frac{\partial\vec{U}_{p_i}}{\partial t}\, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i}\vec{g} - \nabla p - \alpha\vec{l} + \mu\triangle\vec{l}\, d\Omega_{p_i} && \text{in } \Omega_{p_i}\\
&\int_{\Omega_{p_i}} \omega_{p_i}\, d\Omega_{p_i} = \frac{1}{2}\int_{\Omega_{p_i}} \nabla\times(\vec{u} - \vec{U}_{p_i})\, d\Omega_{p_i} && \text{in } \Omega_{p_i}
\end{aligned} \tag{4-16}$$

In addition to the system of equations 4-16, the rigid body constraint, the Lagrange multipliers and the particle advection equations must be included in the complete formulation:

$$
\begin{aligned}
&\vec{l} = 0 && \text{in } \Omega_f \\
&\vec{u} = \vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i}) && \text{in } \Omega_{p_i} \\
&\frac{\partial \vec{X}_{p_i}}{\partial t} = \vec{U}_{p_i} && \text{for } p_i \in (1 \ldots n_p)
\end{aligned}
\tag{4-17}
$$

The formulation proposed in this chapter takes into account the buoyancy forces in each particle and therefore is more adequate to study complex flows with particles that float in the interface of two immiscible fluids. This type of flow will be discussed in the following chapter.

4.3 Variational formulation

To write the system of differential equations stated in the previous section (see Equations 4-16 and 4-17) in a variational form we need to choose the solution space for the physical unknowns related with the problem. The mathematical argumentation in the previous section was based on the fact that the velocity field $\vec{u}$ is constrained to be a rigid–body motion inside particle's domain Ω_p, avoiding its viscous deformations inside the particle's domain Ω_p. A natural choice for solution space of the fluid's velocity and pressure, the Lagrange multipliers field and the particle's velocities is:

$$\mathbb{C} = \{(\vec{u}, p, \vec{l}, \vec{U}_{p_i}, \omega_{p_i}) \,|\, \vec{u} \in \mathbb{V},\ p \in \mathbb{P},\ \vec{l} \in \mathbb{L},\ \vec{U}_{p_i} \in \mathbb{R}^2,\ \omega_{p_i} \in \mathbb{R}\} \tag{4-18}$$

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

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

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

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

From this combined solution space, we can give a different interpretation for the previous strong formulation (Equations 4-16 and 4-17). In our fictitious domain approach the extended formulation over the whole domain is obtained removing the fluid's velocity restriction inside the particles $\vec{u} = \vec{U}_{p_i} + \omega_{p_i} \times (\vec{x} - \vec{X}_{p_i})$ from the combined solution space, and enforcing it as a side constraint. As we saw before, this is done using the Lagrange multipliers $\vec{l}$, which is non–zero only inside the particles and can be interpreted as the traction force required to avoid viscous deformations inside the particles domain Ω_{p_i} and maintain its rigid–body motion.

Observe that the last two equations in the differential formulation of the governing equations (see Equation 4-16) are a differential and an algebraic equation respectively that are used to determine the unknowns $\vec{U}_{p_i}$ and ω_{p_i} and therefore they must be incorporated into the final variational system. The equation for the angular velocity ω_{p_i} (last Equation on 4-16) will be taken without additional mathematical manipulations, while for the particle's velocity equation we will use the divergence theorem in the Laplacian of the Lagrange field, which gives:

$$\int_{\Omega_{p_i}} (\rho_{p_i} - \rho_f)\frac{\partial \vec{U}_{p_i}}{\partial t}\, d\Omega_{p_i} = \int_{\Omega_{p_i}} \rho_{p_i}\vec{g} - \nabla p - \alpha\vec{l}\, d\Omega_{p_i} + \int_{\partial\Omega_{p_i}} \mu\nabla\vec{l}\cdot\vec{n}_{p_i}\, d\partial\Omega_{p_i} \quad (4\text{-}19)$$

The variational formulation for the fluid's momentum and continuity equations for particulate flow problems are almost the same derived on the previous chapter 3 for incompressible flows. The only difference between them is that we need to complete the formulation of the momentum equation of the particulate flow problem with the variational version of the equation that describes the constraint force $\vec{F}$ in terms of the Lagrange multipliers $\vec{l}$.

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. We can write the variational form of the Lagrange multipliers part of the momentum equation as follows:

$$\int_{\Omega} (\alpha\vec{l} - \mu\triangle\vec{l})\cdot\vec{\phi}\, d\Omega \quad (4\text{-}20)$$

If we use the identity:

$$\triangle\vec{l}\cdot\vec{\phi} = \nabla\cdot(\nabla\vec{l}\cdot\vec{\phi}) - \nabla\vec{l} : \nabla\vec{\phi}$$

and the divergence theorem, we can rewrite the equation 4-20 as follows:

$$\int_{\Omega} \alpha\vec{l}\cdot\vec{\phi} + \mu\nabla\vec{l} : \nabla\vec{\phi}\, d\Omega - \int_{\partial\Omega} \mu\hat{f}\cdot\vec{\phi}\, d\partial\Omega \quad (4\text{-}21)$$

where $\hat{f} = \nabla\vec{l}\cdot\vec{n}$ and $\vec{n}$ represents the outward normal to $\partial\Omega$.

The variational version for the governing equations of problems using the fictitious domain method based on Lagrange multipliers can be finally stated in the following way:

Find $\vec{u} \in \mathbb{V}$, $p \in \mathbb{P}$, $\vec{l} \in \mathbb{L}$, $\omega_{p_i} \in \mathbb{R}$ and $\vec{U}_{p_i} \in \mathbb{R}^2$ such that $\forall\vec{\phi} \in \mathbb{H}^1(\Omega)$ and $\forall\chi \in \mathbb{H}^0(\Omega)$:

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

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

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

$$\int_{\Omega_{p_i}} \omega_{p_i}\, d\Omega_{p_i} = \tfrac{1}{2}\int_{\Omega_{p_i}} \nabla \times (\vec{u} - \vec{U}_{p_i})\, d\Omega_{p_i} \quad \text{in } \Omega_{p_i}$$

(4-22)

Observe that 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, see (9).

In addition to the system of equations 4-22 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 particle's advection. The variational form of this last set of equations is straightforward:

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

$$\int_{\Omega_{p_i}} (\vec{u} - \vec{U}_{p_i}) \cdot \vec{\phi}\, d\Omega_{p_i} = \int_{\Omega_{p_i}} \omega_{p_i}(\vec{x} - \vec{X}_{p_i}) \cdot \vec{\phi}\, d\Omega_{p_i} \quad \text{in } \Omega_{p_i} \tag{4-23}$$

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

The momentum and the continuity equations are defined over the whole domain Ω, and that is the reason why the weak formulation can be discretized in space on a single and fixed discretization of Ω, avoiding the need of remeshing around the particles, as we will describe in the next section. Observe that we must only solve the rigid body constraint, the particle's velocity and angular velocity equations inside the region covered by particles. The Lagrange multipliers field must also be solved over the whole domain Ω.

4.4
Fully coupled and implicit discretization

The fictitious domain formulation for simulations of flows with suspended particles described in this thesis allows us to discretize the whole computational domain Ω by means of a single and fixed mesh. As usual, in finite element method, we need to choose the finite dimensional solution space, which will approximate the solution space previously defined in 4-18. Let us say that the finite element solutions are defined to be in the following space:

$$\mathsf{C} = \{(\vec{\mathsf{u}}, \mathsf{p}, \vec{\mathsf{l}}, \vec{U}_{p_i}, \omega_{p_i}) | \vec{\mathsf{u}} \in \mathsf{V}, \mathsf{p} \in \mathsf{P}, \vec{\mathsf{l}} \in \mathsf{L}, \vec{U}_{p_i} \in \mathbb{R}^2, \omega_{p_i} \in \mathbb{R}\} \tag{4-24}$$

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

$$\mathsf{V} := \{\vec{\mathsf{u}} \in \mathbb{P}_4(\Lambda) \times \mathbb{P}_4(\Lambda) \mid \vec{\mathsf{u}} \mid_{\partial\Lambda} = 0\}$$

$$\mathsf{L} := \{\vec{\mathsf{l}} \in \mathbb{P}_4(\Lambda) \times \mathbb{P}_4(\Lambda) \mid \vec{\mathsf{l}} \mid_{\Lambda_f} = 0\}$$

$$\mathsf{P} := \{\mathsf{p} \in \mathbb{P}_2(\Lambda)\}$$

where we used $\mathbb{P}_4$–$\mathbb{P}_2$ elements to build the mesh Λ which approximates the simulation domain Ω. Quadrangular or triangular $\mathbb{P}_4$–$\mathbb{P}_2$ elements have continuous biquadratic interpolation for the velocity $\vec{u}$ and the Lagrange multiplier field $\vec{l}$, and continuous bilinear interpolations for the pressure p approximations. It is well known that $\mathbb{P}_4$–$\mathbb{P}_2$ elements are stable basis functions for solving the Navier–Stokes equations using the finite element method and for this reason we also adopted it on our particulate flow application.

Using this finite dimensional approximation solution space C, we can rewrite the variational formulation for the governing equations 4-22 in the finite element discret fashion, as follows:

Find $\vec{\mathsf{u}} \in \mathsf{V}$, $\mathsf{p} \in \mathsf{P}$, $\vec{\mathsf{l}} \in \mathsf{L}$, $\omega_i \in \mathbb{R}$ and $\vec{U}_i \in \mathbb{R}^2$ such that $\forall\vec{\phi} \in \mathbb{P}_4(\Lambda)$ and $\forall\chi \in \mathbb{P}_2(\Lambda)$:

$$
\begin{aligned}
&\sum_{\tau\in\Lambda}\int_{\tau}\left(\rho_f\frac{\mathrm{D}\vec{\mathsf{u}}}{\mathrm{Dt}}-\vec{g}\right)\cdot\vec{\phi}\,d\tau=\sum_{\tau\in\Lambda}\int_{\tau}(\alpha\vec{\mathsf{l}}\cdot\vec{\phi}-\boldsymbol{\sigma}:\nabla\vec{\phi}+\mu\nabla\vec{\mathsf{l}}:\nabla\vec{\phi})\,d\tau && \text{in } \Lambda\\
&\sum_{\tau\in\Lambda}\int_{\tau}(\nabla\cdot\vec{\mathsf{u}})\chi\,d\tau=0 && \text{in } \Lambda\\
&\sum_{\tau\in\Lambda_{p_i}}\int_{\tau}(\rho_{p_i}-\rho_f)\frac{\partial\vec{U}_{p_i}}{\partial t}\,d\tau=\sum_{\tau\in\Lambda_{p_i}}\int_{\tau}\rho_{p_i}\vec{g}-\nabla\mathsf{p}-\alpha\vec{\mathsf{l}}\,d\tau && \text{in } \Lambda_p\\
&\sum_{\tau\in\Lambda_{p_i}}\int_{\tau}\omega_{p_i}\,d\tau=\tfrac{1}{2}\sum_{\tau\in\Lambda_{p_i}}\int_{\tau}\nabla\times(\vec{\mathsf{u}}-\vec{U}_{p_i})\,d\tau && \text{in } \Lambda_p
\end{aligned}
\tag{4-25}
$$

The discrete version of the rigid body constraint for the fluid's velocity inside the particle's domain and the Lagrange multipliers variational equations are also straightforward:

$$
\begin{aligned}
&\sum_{\tau\in\Lambda_f}\int_{\tau}\vec{\mathsf{l}}\cdot\vec{\phi}\,d\tau=0 && \text{in } \Lambda_f\\
&\sum_{\tau\in\Lambda_{p_i}}\int_{\tau}(\vec{\mathsf{u}}-\vec{U}_{p_i})\cdot\vec{\phi}\,d\tau=\sum_{\tau\in\Lambda_{p_i}}\int_{\tau}\omega_{p_i}(\vec{x}-\vec{X}_{p_i})\cdot\vec{\phi}\,d\tau && \text{in } \Lambda_p\\
&\frac{\partial\vec{X}_{p_i}}{\partial t}=\vec{U}_{p_i} && \text{for } p_i\in(1\ldots n_p)
\end{aligned}
\tag{4-26}
$$

As in chapter 3, the finite element discretization of the variational formulation 4-22 and 4-23 leads to a non–linear system of time–dependent differential equations. Again we will perform the time integration using the implicit Euler method that leads to a system of non–linear algebraic equations. The equations are fully coupled and solved together using Newton's method. The entries of the Jacobian matrix and of the residue vector are presented in Appendix B.

We numerically compute the integrals 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 the particle's domain, since Ω_{p_i} in general is not exactly covered by the mesh elements (see Figure 4.3).

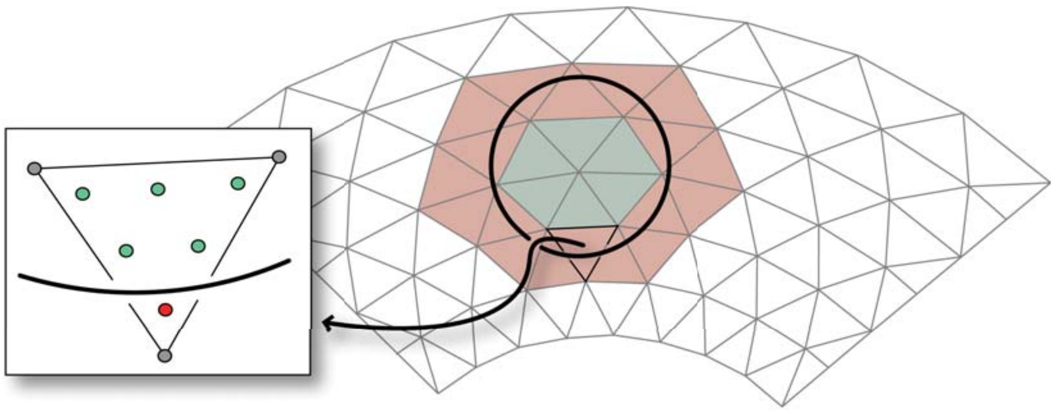

Figure 4.3: Gaussian quadrature: only Gaussian points lying inside the particles p_i are used to integrate over the domain Ω_{p_i}.

In case that the surface of the particle intersects the interior of a given element, we can choose to perform one of the two options: the first approach considers only the Gaussian points that lies inside the particle p_i to perform the integration over Ω_{p_i}, and the second option virtually adapts the mesh around the particle, that is, a mesh refinement is done without changes on the original mesh. The first approach was the integration procedure used on the results that will be presented on the next chapters. This 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 4.4 shows the variation of the area of a particle moving along a finite element mesh. On the example, we used a uniform mesh of square elements, with 9 Gaussian points. The ratio of the elements' area with respect to the particle's area was 0.15 (three first graphs of the figure) and 0.05 (three last graphs of the figure). The first plot on each group shows the approximated area of a particle with 0.0176 cm^2. The second plots shows the absolute approximation error in each time step. Finally, the last graph shows the percentage of the area neglected by the approximation. 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 Chapter 7.

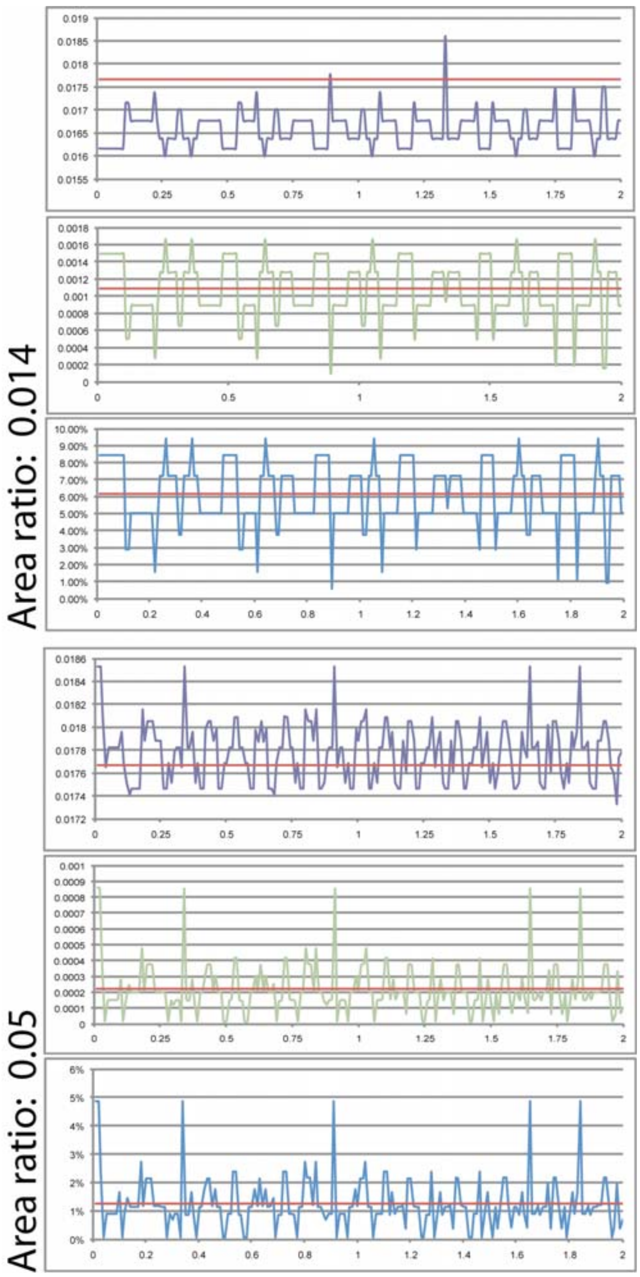

Figure 4.4: Gaussian quadrature: variation of the area of a particle during the simulation time. The first graphs show the results obtained using an area ration 0.014, and the last ones a ration 0.05. In each case, we show the approximated area, the absolute error and the percentage of the analytical area that is neglected by the approximation.