2
Theoretical framework

The aim of this chapter is to review the governing equations for Newtonian incompressible fluids (see section 2.3), the equation of motion of rigid bodies (see section 2.4), and also the capillarity force that acts on particles floating at the interface of two immiscible fluid phases (see section 2.5). Before starting the physical framework description, we establish the notation (see section 2.1) and the system of measurement units (see section 2.2) that will be adopted throughout this text.

2.1
Notations

Consider a two–dimensional bounded simulation domain Ω with external boundary $\partial\Omega$, which is filled with Newtonian incompressible fluids and embedded solid particles. Whenever the context is clear, we call *fluid* one or more immiscible, Newtonian and incompressible fluid phases filling the simulation domain Ω, as illustrated by Figure 2.1.

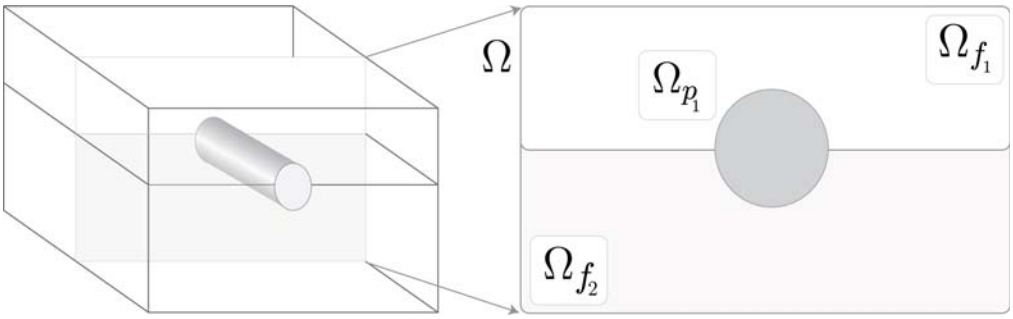

Figure 2.1: Sketch of a simulation scenario: two immiscible fluid phases Ω_{f_1} and Ω_{f_2} filling a 2d box Ω and one embedded particle covering the region Ω_{p_1}.

We denote $\Omega_f = \bigcup_{f_i=1}^{n_f} \Omega_{f_i}$ the region of Ω occupied by n_f fluid phases $f_i \in \{1 \dots n_f\}$ with densities ρ_{f_i} and viscosities μ_{f_i} and we denote $\Omega_p = \bigcup_{p_i=1}^{n_p} \Omega_{p_i}$ the region of Ω covered by n_p rigid particles $p_i \in \{1 \dots n_p\}$ with densities ρ_{p_i} and radius R_{p_i}. We also represent the interface between fluid and particles by $\partial\Omega_p = \bigcup_{i=1}^{n_p} \partial\Omega_{p_i}$, and we denote the interface between two fluid phases f_i and f_j by $\partial\Omega_{f_{ij}}$. Finally, we observe that $\Omega = \Omega_f \bigcup \Omega_p$.

Figure 2.1 sketches a typical simulation scenario composed by a two dimensional simulation domain filled by two fluid phases and one embedded solid particle (right) and its three dimensional representation (left). In the right image we also use the notations previously defined to identify the fluid and particle regions.

A *mesh* Λ is a finite collection of triangles/quadrangles that discretizes the simulation domain Ω. Such collection satisfies the condition that the intersection of two triangles/quadrangles is either empty or a common vertex or a common edge. We call *element*, and denote by τ, each triangle or quadrangle of the mesh Λ. We also denote $\Lambda_f = \bigcup_{f_i=1}^{n_f} \Lambda_{f_i}$ the set of elements belonging to Λ that are completely inside the fluid region Ω_f and by $\Lambda_p = \bigcup_{p_i=1}^{n_p} \Lambda_{p_i}$ the elements of Λ that lies completely or partially inside the particle domain Ω_p, where Λ_{f_i} and Λ_{p_i} are the set of elements inside the fluid phase f_i and the particle with index p_i respectively. Figure 2.2 sketches a mesh discretization of a domain Ω filled by two fluid phases and one embedded solid particle.

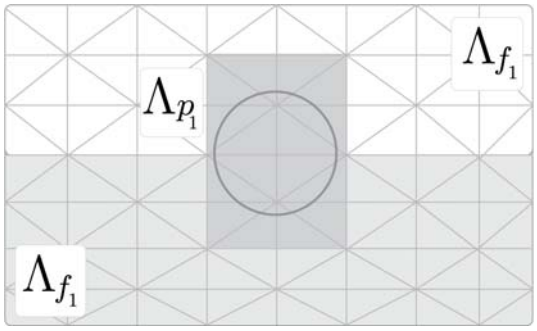

Figure 2.2: Sketch of the regions of a triangulation of the simulation domain.

Observe that, in general, the element sets Λ_f and Λ_p are not disjoint, that is, $\Lambda_f \bigcap \Lambda_p \neq \emptyset$, which indicates that the particle's boundary are not covered by the edges of the elements. Otherwise, if we denote an edge on the mesh by $\epsilon \in \Lambda$, we choose to build the fluid's mesh such that each phase f_i is disjoint to the others or shares a set of edges $\partial\Lambda_{f_ij}$ with each neighbor phase f_j. More precisely, $\Lambda_{f_i} \bigcap \Lambda_{f_j} = \emptyset$ or $\Lambda_{f_i} \bigcap \Lambda_{f_j} = \partial\Lambda_{f_ij}$ if and only if $f_i \neq f_j$.

2.2 System of measurement units

This work adopts a system of units in such a way that the entries of the matrix obtained after the discretization process are of order 1. This reduces numerical instabilities on the simulations that will be later discussed in this work. Such choice shows to be more appropriate to reproduce the scale of some of the real world processes that motivated this thesis, such as coating and drying processes of small particles.

The base measurement units of length, mass and time are centimeters (cm), grams (g) and deciseconds (ds), and its conversion to the International System of Units (IS) is straightforward. To help the reader to interpret the physical parameters and the simulations' results, we show in Table 2.1 some physical constants, such as viscosity and density of water in the IS system and its conversion to the system adopted here.

	International system	Thesis system
Water density	$10^3 \frac{kg}{m^3}$	$1 \frac{g}{cm^3}$
Water viscosity	$10^{-3} \frac{kg}{m \cdot s}$	$10^{-3} \frac{g}{cm \cdot ds}$
Water/air tension	$70 \frac{kg}{s^2}$	$0.7 \frac{g}{ds^2}$
Gravity force	$10 \frac{m}{s^2}$	$10 \frac{cm}{ds^2}$

Table 2.1: Physical constants converted from SI to our system of units.

2.3 Navier–Stokes equations

The Navier–Stokes equations model the laminar flow of compressible and incompressible fluids. Those equations are mathematically complex and because of that, their theoretical analysis is difficult and the derivation of general analytical solutions is only possible in very few situations. In this thesis we will only deal with a special class of fluids known as *Newtonian incompressible fluids* which, for example, includes the water.

The Navier–Stokes equations are derived from the physical laws of mass, momentum, and energy conservation. Before reviewing the physical conservation laws, we must define the concept of control volume. A *control volume* $\mathcal{V}$ is a continuum mass without holes, on which the physical conservation laws can be applied. It can remain fixed in space or change its position. These two approaches result in different descriptions for the Navier-Stokes equations: the Eulerian and Lagrangian formulations. The Eulerian formulation, which is adopted in this work, uses a spatial description, where $\mathcal{V}$ is fixed in space, while the Lagrangian approach uses a material description, where $\mathcal{V}$ moves along with the fluid (see Figure 2.3). If the control volume moves along with the flow, there is no mass flow across its boundary, and the mass inside it is constant. In this particular case, the control volume is called a system.

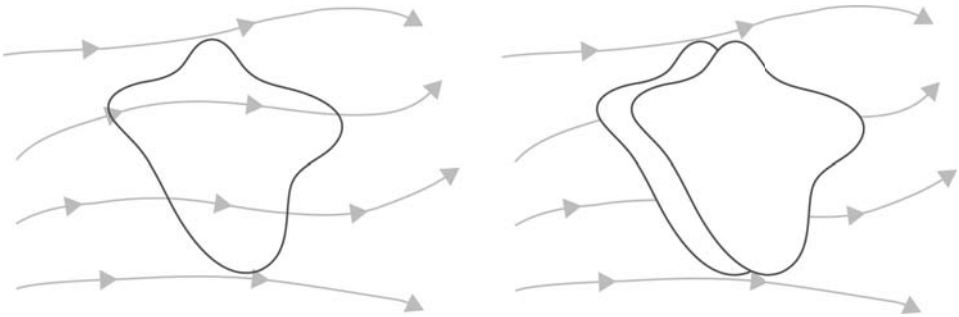

Figure 2.3: Eulerian (left) and Lagrangian (right) control volumes.

Using the control volume concept, we can now state the conservation laws of mass, momentum and energy:

1. **Mass conservation**: In the absence of sources or sinks of mass (for which the local mass may disappear), the mass that enters a control volume $\mathcal{V}$ must leave and/or accumulate inside it. The *continuity equation* mathematically describes this principle.

2. **Momentum conservation**: The rate of change of momentum of the control volume $\mathcal{V}$ is equal to the net force acting on it. This physical principle is also known as the Newton's second law, and its mathematical description is called the *momentum conservation equation*.

3. **Energy conservation**: The principle of conservation of energy says that in an isolated system, the internal energy remains constant. This principle comes from the first law of the thermodynamics and the resulting equation is called *energy conservation equation*.

For all physical simulations that we will study through this thesis, we write the governing momentum and mass conservation equations as follows:

$$\rho_{f_i} \frac{\mathrm{D}\vec{u}_{f_i}}{\mathrm{Dt}} = \nabla \cdot \boldsymbol{\sigma}_{f_i} + \vec{g} \quad \text{in} \quad \Omega_{f_i} \tag{2-1}$$

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

where the external body forces, like the gravity force, is denoted by $\vec{g}$, the subscript f_i represents the index of the fluid phase inside the region Ω_{f_i}, the vector field $\vec{u}_{f_i}$ is the phase's velocity and $\boldsymbol{\sigma}_{f_i}$ is the stress tensor for Newtonian fluids, which is written as:

$$\boldsymbol{\sigma}_{f_i} = -p_{f_i}\boldsymbol{\delta} + \mu_{f_i}(\nabla\vec{u}_{f_i} + \nabla\vec{u}^t_{f_i}) \tag{2-3}$$

where p_{f_i} is the phase pressure and $\boldsymbol{\delta}$ the identity tensor.

The operator $\frac{D*}{Dt}$ denotes the *material derivative* which physically describes the rate of change of a quantity measured by an observer moving with the fluid, and is defined as:

$$\frac{\mathrm{D}*}{\mathrm{Dt}} = \frac{\partial *}{\partial t} + \vec{u} \cdot \nabla * \tag{2-4}$$

where the first term is the *local derivative*, while the second one represents the variation due to the flow and is called *convective derivative*.

A detailed discussion on the Navier–Stokes equations can easily be found in the literature, for example in the works (5, 7, 30, 39).

2.4 Rigid body motion

We can define a *rigid body* as an ideal body or solid such that the relative distances between all material points do not change, even under the action of an external force. The motion of a rigid body can always be decomposed in translations and rotations. When a rigid body is translated, its material points describe parallel trajectories and, when we rotate a solid body, all material points describe concentric circles (see Figure 2.4).

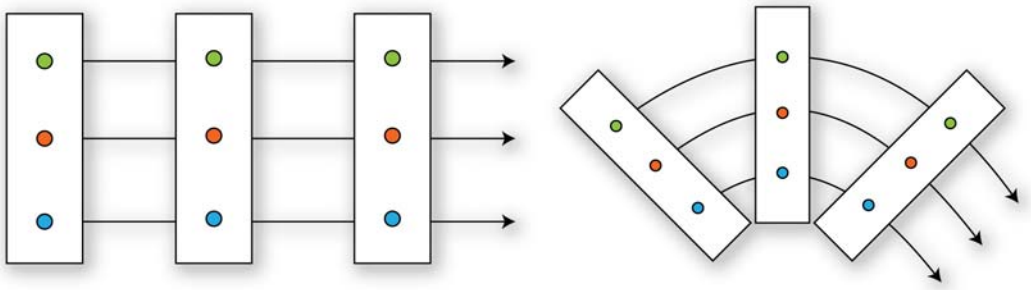

Figure 2.4: Rigid body motion: a translation (left) and a rotation (right) of a rigid bar. The material points describe parallel and concentric trajectories.

Let us denote the translational velocity, or only velocity for simplicity, of the centroid $\vec{X}_{p_i}$ of a particle p_i by $\vec{U}_{p_i}$ and its angular velocity by ω_{p_i} with $p_i \in \{1 \dots n_p\}$. The rigid body motion equations for the translational and angular velocities of a rigid particle embedded in a fluid can be written as:

$$M_{p_i} \frac{\partial \vec{U}_{p_i}}{\partial t} = M_{p_i} \vec{g} + \vec{H}_{p_i} \quad \text{in} \quad \Omega_{p_i} \tag{2-5}$$

$$\mathbf{I}_{p_i} \frac{\partial \omega_{p_i}}{\partial t} + \omega_{p_i} \times \mathbf{I}_{p_i} \omega_{p_i} = \vec{T}_{p_i} \quad \text{in} \quad \Omega_{p_i} \tag{2-6}$$

where M_{p_i} is the mass of the particle, $\vec{H}_{p_i}$ is the hydrodynamic force acting on the particle, $\mathbf{I}_{p_i}$ is its inertial tensor and $\vec{T}_{p_i}$ is the hydrodynamic torque about its center of mass.

2.5
Capillarity force

It is frequently observed that particles floating on a liquid interface are submitted to forces which in most cases tend to produce clusters of particles (6, 14, 17, 24, 26, 27, 33, 34, 42). These particles may be either attracted to a wall or to each other. The attraction occurs because a concave meniscus is formed between the particles if they are close enough (the interaction force increases exponentially when the distance between particles decreases).

The concave meniscus creates a region of sub–ambient pressure underneath it, leading to a net surface force that pulls the particles together. Moreover, the concave meniscus also leads to a non–uniform line force along the contact line between the interface and the particle surface, which may also pull the particles together. The direction of the force may be the opposite, i.e. the particles are pushed apart, if the wetting characteristic of the particle surface is such that a convex meniscus is formed.

Figure 2.5 sketches the capillarity effects between two particles. The images at the first row show the non–uniform force acting along the contact line between the particle surface and the interface. If we denote the ambient and two different underneath meniscus pressures by p_a, p_1 and p_2, the second row on the image shows the pressure configuration due to the interface deformation.

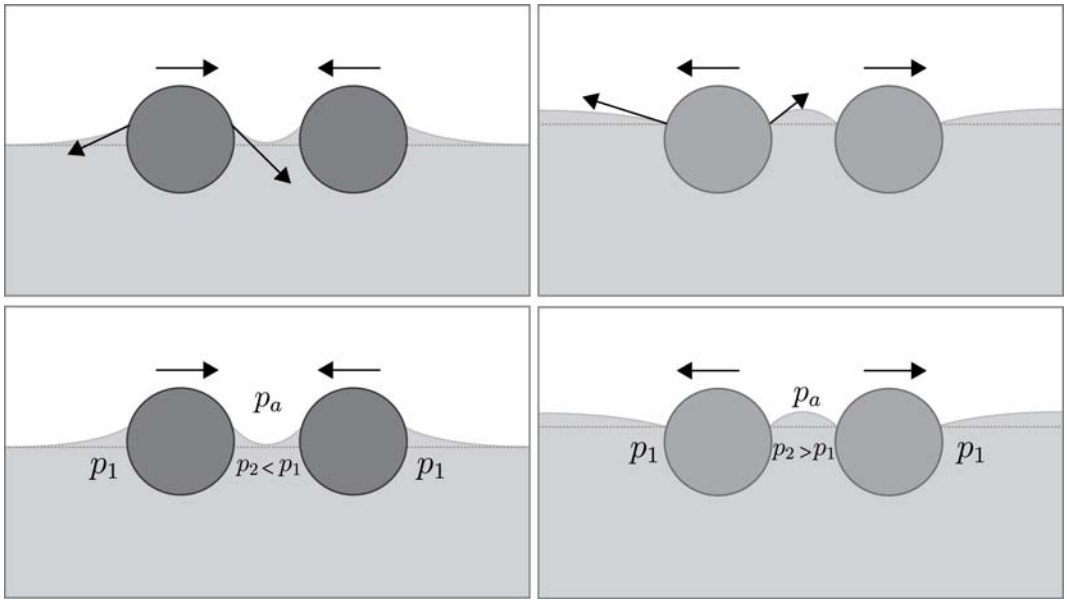

Figure 2.5: Attraction (left) and repulsion (right) behaviors of the lateral capillarity force between two particles on a liquid interface.

When a single particle is floating at the fluid interface, or when a particle has no neighbors close enough, the horizontal component of the capillarity force

cancels along the contact line between the interface and the particle surface. In this case, only the vertical component of the capillarity force acts on the floating particle (see Figure 2.6). The vertical component of the capillarity force, together with the gravity and buoyancy forces, determine the immersed height of a particle in rest.

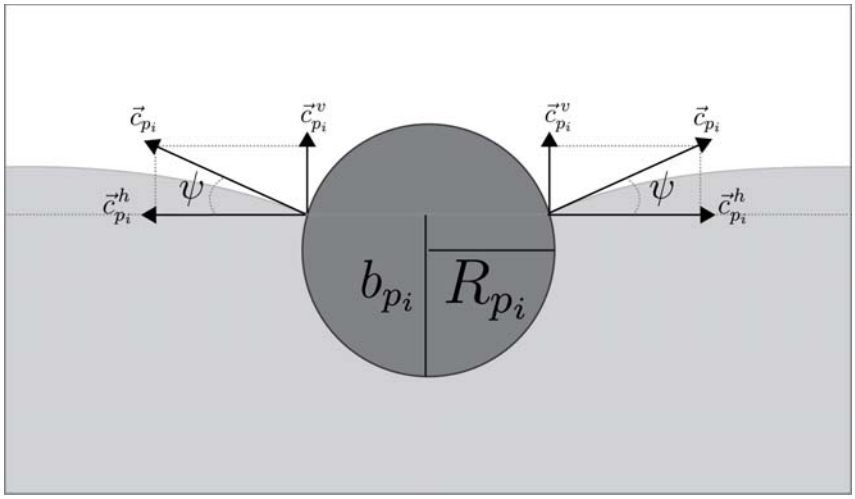

Figure 2.6: Sketch of the capillarity force acting on a floating particle and the parameters related with the body force approach.

We denote by $\vec{c}_{p_i}$ the capillarity force acting on a particle p_i floating on the interface between two fluid phases. The horizontal and vertical components of the capillarity force are denoted by $\vec{c}^{\,h}_{p_i}$ and $\vec{c}^{\,v}_{p_i}$ respectively. Using the body force approach, they are written as:

$$\vec{c}^{\,h}_{p_i} = 2\varsigma \cos(\arccos(\frac{b_{p_i}}{R_{p_i}}) - \psi) \tag{2-7}$$

$$\vec{c}^{\,v}_{p_i} = 2\varsigma \sin(\arccos(\frac{b_{p_i}}{R_{p_i}}) - \psi) \tag{2-8}$$

where ς represents the surface tension at the phases' interface $\partial\Omega_{f_{ij}}$, and ψ denotes the contact angle between the particle and the lower fluid phase. The value b_{p_i} denotes the immersed height of the particle, and as defined before R_{p_i} is the particle radius (see figure 2.6).

One contribution of this work is the development of a numerical method to simulate the action of flotation forces and the clustering process of floating particles. In our formulation, we model the capillarity force as an external body force acting directly on the particles as described by Kralchevsky et al (2001) (25). The great advantage of this approach is that we can avoid the simulation of interface deformations, which makes easier the development of the floating particles algorithm.