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Numerical studies of the sloshing phenomenon using the Smoothed Particle Hydrodynamics (SPH) method.

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‘Nothing in life is to be feared, it is only to be understood.
Now is the time to understand more, so that we may fear less.’

Marie Curie

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Abstract

The purpose of the present thesis is to increase the applicability of Smoothed Particle Hydrodynamics (SPH) method to sloshing problems relevant in engineering.

The thesis is structured around three main topics: theoretical improvements on SPH, implementation of tools and physical models within the open-source software AQUAplusph, and studies on 3-D geometries and application cases.

The theoretical aspects of the method which are considered crucial for sloshing flows are analyzed. Particular attention is paid to boundary conditions, and more specifically, to the approaches developed to deal with solid boundaries. A novel general formulation to compute the Shepard renormalization factor operator used within the boundary integrals methodology is developed. This allows for improved simulations of hydrostatic problems, reducing spurious motions induced at the free surface and improving accuracy near the boundary. Additionally, the conservation properties of the boundary integrals formulation are studied. Momentum conservation is assessed through a new methodology that links volume and surface integrals through generalized coordinates, and the energy balance in the boundary integrals framework is also presented. Verification of the novel formulations are assessed by means of a hydrostatic test and the motion of a body inside a fluid.

These novel formulations have been added into the open-source code, AQUAplusph. Moreover, a set of tools and physical models have been included in the set of capabilities available within the code: tools to improve particle initialization and free-surface tracking have been adopted and extended to a boundary integrals formulation. A set of physical models that have been identified as relevant improvements for sloshing flows have also been implemented. In particular, a turbulent Large Eddy Simulation (LES) model and phase change are incorporated into the code.

Several benchmark test cases are performed in order to demonstrate the benefits of the novel implementations: a dam-break and a moving square inside a fluid have been extensively analyzed to compare new approaches versus standard formulations.

Finally, theoretical additions and numerical implementations are tested and applied to three relevant engineering applications: a 3-D dam-break, an anti-roll tank of a seagoing ship and a vertical sloshing fuel aircraft tank. The 3-D dam-break shows how impact pressures computed

at the wall with the novel boundary formulation are in accordance with state-of-the-art results obtained with SPH and with experimental data for the same problem, regardless of resolution. Simulations on the vertical motion of a tank filled with liquid have been carried out for different motion models, including a coupling with a Euler-Bernoulli beam model. Results demonstrate that SPH is a valid method for modeling damping forces due to fluid motion in liquid sloshing. This may open opportunities for using this effect to reduce turbulence-induced motions in aircraft wings.

Resumen

El propósito de esta tesis es incrementar el rango de aplicación del método de partículas *Smoothed Particle Hydrodynamics (SPH)* a problemas de ingeniería en los que el fenómeno de *sloshing* es una parte determinante en su diseño.

La tesis está estructurada en torno a tres temáticas principales: mejoras en los aspectos teóricos del método SPH, implementación de herramientas y modelos físicos en el software libre AQUA-gpusph, y estudios en geometrías 3-D y casos de aplicación.

Se han analizado los aspectos teóricos del método SPH que se consideran relevantes para el estudio del problema de *sloshing*. En concreto, se ha hecho énfasis en el estudio de las condiciones de contorno y, de forma más específica, en las diferentes metodologías que se han desarrollado en las últimas décadas para afrontar este problema en paredes sólidas. Se ha desarrollado una nueva formulación para calcular el factor de renormalización de Shepard, dentro de la metodología de integrales de contorno. De esta manera, se consigue mejorar la simulación del problema hidrostático, ya que se reducen los movimientos espúreos que aparecen en la superficie libre, así como se consigue una mejora en la precisión cerca del contorno.

Además, se estudian las propiedades de conservación de la metodología de integrales de contorno. La conservación de momento se consigue a través de una metodología novedosa que interrelaciona integrales de volumen y de superficie mediante coordenadas generalizadas. Por otro lado, se desarrolla la ecuación de balance de energía en el contexto de las integrales de contorno.

Todas estas formulaciones novedosas se han añadido al código libre y abierto AQUA-gpusph. Además, se han incluido una serie de herramientas y modelos físicos dentro de las capacidades del código: las herramientas implementadas se centran en la mejora de la disposición inicial de partículas y la identificación de partículas de superficie libre, que se han adaptado desde otras metodologías a la metodología de integrales de contorno. Se han implementado así mismo una serie de modelos físicos que se han considerado relevantes para el estudio de los problemas de *sloshing*. En concreto, se han incorporado un modelo de turbulencia LES, y un modelo de cambio de fase.

Se han llevado a cabo una serie de casos de validación para demostrar las mejoras incluidas con las nuevas formulaciones: la rotura de una presa, y el movimiento de un objeto cuadrado

dentro de un fluido se han analizado de forma extensiva, comparando los resultados obtenidos con las formulaciones estándar del método.

Finalmente, las mejoras teóricas y las implementaciones numéricas anteriormente descritas se han aplicado a tres aplicaciones relevantes para la ingeniería: una rotura de presa en 3-D, el tanque de balance de un buque, y el movimiento vertical de un tanque de combustible de un avión. La rotura de presa 3-D muestra cómo las presiones de impacto que se calculan en la pared con la nueva formulación están de acuerdo con otros resultados obtenidos para el mismo problema, tanto experimentales como numéricos, para un rango amplio de resoluciones.

Se han realizado simulaciones del movimiento vertical del tanque de combustible para distintos modelos de movimiento, incluyendo un acoplamiento con una solución basada en el modelo de Euler-Bernoulli. Los resultados obtenidos demuestran que SPH es un método válido para calcular el amortiguamiento añadido que se debe al movimiento del fluido. De esta forma, se puede analizar este efecto de amortiguamiento para reducir los movimientos en las alas de avión debidos a cargas externas.

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Finally, I want to say a word to Victor and Miguel. We are only a few, but with the strongest ties.

Nomenclature

Symbols

$\boldsymbol{g}$	Generic external volumetric force field
$\boldsymbol{n}$	Normal component to boundary condition
$\boldsymbol{r}$	Particle position
$\boldsymbol{u}$	Flow velocity
Δt	Time step
Δx	Discrete particle distance
$\frac{D}{Dt}$	Lagrangian Derivative
γ	Shepard renormalization factor
κ	Thermal conductivity
λ	Viscosity coefficient. Eigenvalue of renormalization matrix.
$\mathbb{D}$	Rate of strain tensor
$\mathbb{T}$	Stress tensor of a Newtonian fluid
μ	Dynamic viscosity
ν	Kinematic viscosity
Ω	Generic fluid domain
$\partial\Omega$	Boundary of generic fluid domain

ρ	Fluid Density
ρ_0	Reference density
$\langle \nabla \rho \rangle_i^L$	Renormalized density gradient
ε_C	Compressible energy
ε_k	Kinetic energy
ε_M	Mechanical energy
ε_p	Potential energy
c_p	Specific heat at constant pressure
c_s	Speed of sound
dr	Particle spacing
h	Smoothing length
m_i	Mass of particle i
Ma	Mach number
p	Pressure
p_a	Atmospheric pressure
q	Normalized particle distance
s	Compact support
T	Temperature
V_i	Volume of particle i
$W(\mathbf{x} - \mathbf{y}, h)$	Kernel function

Abbreviations

ALE Arbitrary Lagrangian Eulerian

AMR Adaptive Mesh Refinement

APR Adaptive Particle Refinement

ART Anti-Roll Tank

BC Boundary Condition

BE Boundary Element

BI Boundary Integrals

CEHINAV Canal de Ensayos Hidrodinámicos Navales

CFD Computational Fluid Dynamics

CFL Courant Friedrichs Levy condition

CPU Central Processing Unit

DEM Discrete Element Method

EOS Equation of State

FDM Finite Difference Method

FEM Finite Element Method

FFT Fast Fourier Transform

FS Free Surface

FVM Finite Volume Method

GP Ghost Particles

GPU Graphical Processing Unit

IC Initial Condition

ISPH Incompressible Smoothed Particle Hydrodynamics

LES Large Eddy Simulation

LNG Liquefied Natural Gas

MLS Moving Least Squares

MPS Moving Particle Semi-Implicit

PFEM Particle Finite Element Method

PIC Particle In Cell

SPH Smoothed Particle Hydrodynamics

TLD Tuned Liquid Damper

VBPM Virtual Boundary Particle Method

VOF Volume of Fluid

WC-SPH Weakly Compressible Smoothed Particle Hydrodynamics

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Chapter 1

Introduction

The present thesis covers the study of liquid sloshing from a numerical perspective, using a mesh free based method known as Smoothed Particle Hydrodynamics (SPH).

1.1 Motivation

1.1.1 General

Sloshing is defined as the motion of liquids inside partially filled containers. Even though sloshing can be non-violent, and even linear, this work's context is that of confined flows in complex geometries, in which violent impacts, high fragmentation of the free surface and highly non-linear fluid dynamics are present. Complex physics, including effects of turbulence, thermodynamics or hydro-elasticity have not been studied in depth in the literature and will be investigated herein.

From an engineering point of view, sloshing is in general a non-avoidable effect that sometimes can be used in certain applications to dampen or control motions induced by external forces. Successful examples of controlled sloshing can be found in the literature for many fields, such as:

- LNG carriers: control refers here to the search of the optimal configuration, which consists of octagonal tanks that maximize payload over other options such as spherical (MOSS)

tanks. However, sloshing needs to be studied in depth for each design [Gavory and Seze, 2009].

- Anti-roll tanks (ART): designed to generate a counter-moment that is aimed to dampen (minimize) roll motions in certain types of ships, such as fishing or oceanographic vessels. This is a successful example of a useful application of sloshing [Souto-Iglesias et al., 2006].
- Tuned Liquid Dampers (TLD), used to reduce motions in buildings and structures due to earthquakes. Their working principle is based on increasing the effective damping characteristics of the structure, thus becoming another successful example of sloshing applied to engineering problems. [Bulian et al., 2010, Bouscasse et al., 2014a,b].
- Vertical motion in aircraft wings: this is another example in which sloshing can be used to minimize motion by adding a substantial damping in certain conditions that need to be studied mainly for fuel storage tanks [Shreeharsha et al., 2017].
- Sloshing in propellant rocket tanks, that incorporate vents used to generate motion and orientate the rocket in space. The sloshing flow affects to several physical phenomena such as phase change, becoming in turn important for the effectiveness of the motion control thrusters. Hence, here sloshing is not used but has to be controlled, to reduce its negative effects [Alexander and Lundquist, 1988].

Regardless the application, violent sloshing lead to structural damages or dangerous motions, even in the cases where it is used to reduce them. That is why an accurate and precise study of sloshing loads and resultant motions is critical in several engineering applications such as the ones presented above.

It is in the fifties and the sixties when the sloshing problem gained attention from the research community. Preliminary studies taking advantage of sloshing in different disciplines can be found for example in the works of Graham and Rodriguez [1951], Housner [1957], Abramson et al. [1966] or Van Den Bosch and Vugts [1966]. Research on the problem has progressed in the last 50 years, and general reviews analysing linear and non-linear sloshing from a general perspective can be found in the works of Ibrahim [2005] and Faltinsen and Timokha [2009].

From a numerical perspective, first attempts were based on equivalent mechanical system analogies [Graham and Rodriguez, 1951, Lewison, 1976] that were valid to obtain an estimate of the effects of fluid inside moving containers. A more sophisticated theory to obtain fluid action was later developed, based on solving a potential flow problem combined with modal analysis wave theory to obtain free surface shape and evolution [Faltinsen and Timokha, 2009]. Despite the complexity of the theory, this technique cannot handle problems that involve either breaking waves nor complex geometries.

As CFD techniques advanced, a set of methodologies that are popular to analyze sloshing have been developed in recent decades, linked also to the increasing power of computers. These techniques have in common the approximate solution of the Navier-Stokes equations, that are a system of nonlinear equations that can be solved by different means. A review of numerical simulations involving sloshing can be found for example in Rebouillat and Liksonov [2010]. Among the different possibilities, two approaches are normally distinguished:

On one hand, mesh-based methods are a traditional well established approach to sloshing and, in fact, a lot of information related to various engineering problems (including sloshing) can be easily found. In order to track free surface, different approaches have been developed. Some examples are the Level Set Method [Sethian, 1996] and the Volume of Fluid (VOF) method [Hirt and Nichols, 1981]. Both are mainly based on applying a function over an Eulerian grid to get the free surface shape. Although widely used, they have also a set of inconveniences, in particular, numerical diffusion at the interface, that can result in a poor definition of the free-surface in advection dominated flows, leading to issues of mass conservation in fragmented flows. On the other hand, in the last few decades alternative approaches, based on a Lagrangian perspective, have been developed. Among them, Smoothed Particle Hydrodynamics has become popular for free surface flows where high fragmentation of the free surface occurs.

The main advantage of the latter comes from the fact that the free surface treatment is natural, this is, there is no need to define free surface boundary conditions, as they are naturally fulfilled.

On the negative side, SPH is still a relatively young methodology that still needs to be improved in terms of consistency, accuracy and applicability.

Another important development that has made it possible for SPH to be a competitive alternative regarding industrial application is linked to the huge development of hardware facilities with big CPU clusters available all along the world. Also, linked to advances in graphics computing, cinema and video-game industries, GPU computing has arisen as a potential alternative for SPH code development, that, due to its particular algorithm characteristics, is a suitable candidate for such devices. A set of successful commercial and academic SPH codes using this technique can be found in the literature, such as DualSPHysics [Crespo et al., 2015] or AQUAplusph [Cercos-Pita, 2015].

From the academic perspective, it is important that the tools developed comply with a set of requirements. One of the critical aspects is that the knowledge created and made explicit through code development is to be free and accessible to the whole research community. Following this thinking, a fully free open-source tool is used here to develop the methodology. AQUAplusph becomes therefore the ideal candidate for this thesis, as it is an open-source software developed by Cercos-Pita at CEHINAV group during his own PhD thesis [Cercos-Pita, 2016].

Finally, it is important to outline that no single method is currently capable of dealing with the full range of physical problems required for the study of sloshing. This work aims to put another stone towards a better understanding of liquid sloshing.

This introduction is general to the thesis. A more detailed description of the state of the art of each of the topics covered will be given in the corresponding chapters.

1.1.2 Liquid sloshing phenomenology

Liquid sloshing depends of various aspects that influence the intensity, repeatability and duration of sloshing loads. Of course, general considerations such as the type of external loads, their amplitude and frequency, or the container shape and location with respect to the center of gravity of the structure in which the container is set have an influence. However, the most prominent aspects to be considered in order to avoid large sloshing loads are the filling ratio (see Figure 1.1 for an example) and the fluid properties.

Linked to the latter, sloshing can also be influenced by physical conditions and the surrounding

Figure 1.1: Relation between impact pressure and filling level in a LNG tank. source: LRS [May, 2009]

environment, such as pressure and temperature, gas-vapor properties and structural properties.

All in these have a principal consequence, which is that sloshing can be affected by different phenomena. These have been largely studied from the experimental point of view at different conditions (see e.g. Souto-Iglesias et al. [2006], Lafeber et al. [2012], Ludwig et al. [2013], Bulian et al. [2014], Delorme et al. [2009], Arndt [2011], Karimi et al. [2013])

However, it is normally difficult to predict the actual values of the forces due to impacts occurring on the tank walls as a consequence of sloshing, mainly due to its stochastic behavior. Such a difficulty leads to a set of safety requirements that typically overestimate the influence of sloshing, which have direct effect on the design and cost estimates of projects that have to consider this aspect. The complexity of the phenomena involved makes the possibility of modeling the complete physics of an actual sloshing impact load far from being feasible with the experimental approach nowadays.

To better understand the physics inside a sloshing event, the physical phenomena involved can be separated and classified into relatively simple elements [Lafeber et al., 2012]. These elementary processes may have more or less relative importance depending on the particular characteristics of the flow studied, but there are some ideas that are to be considered to understand the problem.

There is in general a strong contribution from the quick change of momentum happening

when a liquid reaches a wall. Associated to this phenomenon, there is also an influence of the momentum transferred from the gas surrounding the liquid that escapes from the gap in between the liquid and the wall. Moreover, it has been reported that liquid-gas density ratio plays a role [Braeunig et al., 2009]. If this ratio is relatively high, compressibility of the gas phase might be important, acting like a cushion that dampens the effect of liquid momentum change contribution [Godderidge et al., 2009]. On the other hand, if this ratio is low, there is little contribution from the gas phase and therefore acoustic waves linked to the liquid phase are important [Brosset et al., 2013]. Finally, there are very specific contributions that largely depend on the conditions in which sloshing happens. Normally, walls on which impacts happen are considered as rigid boundaries that do not deform with the impact, and therefore, they do not absorb any kind of energy that might be transferred from the fluid. Depending on the materials used, this aspect can be considered critical, especially from a structural and fracture point of view. There might be also an influence coming from thermal effects. If liquids are carried out in thermodynamic equilibrium, as it is the case of LNG or launching rocket tanks, phase change might need to be considered, as it might influence the behavior of gas pockets resulting from impacts and/or wave breaking.

With all this in mind, it can be seen that phenomenology associated to impact loads occurring inside partially filled tanks is wide, varied and complex, making it difficult to reproduce all these conditions with a single experimental setup or even a numerical simulation.

The approach is then to study the different aspects separately, isolating the consequences associated to each phenomenon.

1.1.3 State of the art of SPH

SPH is a fully Lagrangian CFD method to solve conservation equations in fluids in differential form. The method was born in 1977 in the context of astrophysics [Gingold and Monaghan, 1977, Lucy, 1977]. However, it started to spread quickly over other disciplines, and in 1994 we can find the first application to fluid dynamics and free surface flows [Monaghan, 1994]. The Lagrangian nature of the method, in the same fashion as other Lagrangian approaches

(PIC, PFEM, MPS, etc.) makes it an attractive solution for flows dominated by the presence of complex geometries or large fragmentation of the free surface.

Focusing on the SPH framework applied to free surface flows, two main approaches can be found, depending on the method used to impose incompressibility: first, the Weakly Compressible (WC-SPH) approach, that is based on the original formulation proposed for astrophysics. It consists on a compressible formulation of the Navier-Stokes equations, in which pressure and density are linked through a stiff Equation of State. Second, there is an incompressible approach (ISPH), based on solving a Poisson equation in order to close the system (pressure-velocity link), in the same fashion as traditional incompressible methodologies.

Although it has been criticized due to the explicit time marching scheme, that results into small time steps and therefore into a computationally expensive scheme, as well as stability issues and a noisy pressure field, the WC-SPH solution does not require any special treatment of the free surface, as this boundary condition appears naturally into the scheme. Also, as it has been already introduced in the previous section, the development of massive parallel codes and the introduction of GPU computing techniques into SPH makes it possible to deal with with small time steps and therefore use this approach competitively.

The use of SPH in multiple contexts has implied that the community has grown exponentially in the last few years, and with it, the different methodologies developed to treat a number of numerical challenges. Indeed, in order to identify and strength these challenges, the SPH community, grouped under SPHERic ERCOFTAC SPH special interest group, has established five main areas for the method to improve and move forward, known as the Grand Challenges. All five challenges are a perfect introduction to the directions in which the researchers should point to. First grand challenge deals with convergence, consistency and stability of the method, which is a key aspect of any numerical method. Although SPH lacks a fully rigorous mathematical formalism in this regard, some work has been done in the past years.

Concerning stability, pairing instability, that used to be a problem in the past recent, has been overcome through the introduction of Wendland kernels [Wendland, 1995] and demonstrated by Dehnen and Aly [2012]. Tensile instability was addressed early in the development of the method [Swegle et al., 1995], introducing a corrective term into the momentum equation, as in

Monaghan [2000] or Colagrossi [2005], or by a modification of the SPH operators depending on pressure field value at an interpolation point [Sun et al., 2018].

Particle redistribution techniques, such as Lind et al. [2012] or Sun et al. [2019a] ones also help reaching stability. Finally, another popular possibility consists on introducing numerical diffusion, normally through artificial viscosity [Monaghan and Pongracic, 1985], but also through Riemann-SPH, a formulation that was introduced by Vila [1999].

With respect to convergence, particle redistribution techniques are also very helpful. SPH can reach good levels of convergence rates if particle ordering is kept. As soon as particle disordering becomes an aspect of the problem studied, SPH convergence rates quickly diminish. Finally, consistency is linked mostly to a correct implementation of boundary conditions [Macia et al., 2011], in itself one of the five grand challenges.

The problem of modeling in a fully Lagrangian framework arise as another key aspect that has been largely studied but that is still an open question. In particular, solid boundary edges (such as the ones that are needed for tank walls) represent a great challenge that has been studied from various perspectives in the last three decades. A thorough review of the different methodologies used to model solid boundaries will be given in Section 3.3 Among these methodologies are the use of boundary integrals (BI), whose implementation is in reality the result of particular normalization techniques for the SPH operators. The use of this BI approach will be one of the central aspects considered in this thesis for the application of SPH to sloshing problems.

Adaptivity is related to the capabilities of SPH for dealing with different particle sizes. This aspect can turn critical when seeking a reduction in overall time cost while maintaining a high level of accuracy at certain areas of the domain. Variable resolution has been introduced in the astrophysical context for SPH years ago [Gingold and Monaghan, 1982], through variations in the kernel size according to density field. Those changes occurred slowly in large domains. Unfortunately a similar approach cannot be followed when extending these models in a weakly-compressible context, as in these cases density must remain nearly constant. Nonetheless, recently a number of approaches have been developed, either consisting of initial regions of different size [Bonet and Rodríguez-Paz, 2005, Oger et al., 2005] or procedures to dynamically

increase or reduce particle size (particle splitting and coalescing procedures) [Vacondio et al., 2013, Barcarolo et al., 2014]. Lately, an Adaptive Particle Refinement (APR) methodology has been used by Chiron et al. [2018] and Sun et al. [2018], based on the use of different layers that cover the fluid domain through a disjoint partition.

Despite the improvements, major challenges are still to be addressed, mainly linked to achieving a full automation dynamic process, in the same fashion as Adaptive Mesh Refinement (AMR), as well as to solving accuracy and robustness issues of the particle refinement methodologies.

A different option to overcome SPH weaknesses and take advantage of its strengths is to use SPH there where it is a powerful method and use a different method to solve a different physics or location of the problem. The coupling between SPH and the other methods is the topic that the fourth grand challenge deals with. The complexity of the coupling algorithm depends on many parameters such as: the type of coupling; the heterogeneity of the methods coupled; the approach (Lagrangian vs Eulerian) of methods; the time stepping or the preservation of elemental properties. Several works can be found in this regard coupling SPH to different methods such as SPH-FEM (e.g. Fourey et al. [2017]), SPH-DEM (e.g. Canelas et al. [2017]), SPH-FDM (e.g. Verbrugghe et al. [2018]), including external coupling in which motion response is influenced by the SPH solution [Camas et al., 2017, Bulian and Cercos-Pita, 2018]. Lately, coupling has been extended to more complex approaches, such as the standard mesh-based Finite Volume Method (FVM) and SPH (see e.g. Marrone et al. [2016], Kumar et al. [2015]), which is a promising approach to take advantage of FVM in problems dealing with complex fluid interfaces.

Finally, there is an important impulse to bring SPH into industrial contexts. Therefore, Grand Challenge number five focuses on the applicability of the method to actual engineering problems. In order to have an impact on industry, pre- and post-processing tools or the ratio between computational cost and precision are definitely aspects to have a look at.

As a matter of fact, SPH has already demonstrated to be a competitive method for different industrial applications. There exists a comprehensive review on successful applications simulated with SPH that has been carried out by Shadloo et al. [2016]. Within this group, applications dealing with e.g. aquaplaning [Hermange et al., 2019], fluid motion in gearboxes [Ji et al., 2018]

or wave-structure interaction [Domínguez et al., 2013] can be found.

1.2 Objectives

The general goal of the present thesis is to make a step forward in the application of SPH to sloshing problems. To achieve this purpose, a number of specific objectives are set:

1. Gain insight into the challenges associated to the SPH method, with emphasis on the boundary conditions approaches for modeling walls as the domain edges.
2. Develop a new kernel formulation to reduce consistency issues for the boundary integrals formulation when free surfaces and boundaries are present in the interpolation.
3. Investigate conservation properties of the SPH method: analyze momentum conservation within a confined boundary perspective and develop the energy balance equation for a boundary integrals methodology.
4. Improve the capabilities of the open-source SPH software AQUAplusph: implementation of all the proposed formulations used throughout this thesis, including pre- and post-processing tools.
5. Expand the physics involved in SPH modeling of sloshing flows: addition of a turbulence LES based model and a phase change model.
6. Apply the improvements found to various application cases within the naval and aerospace industry: a 3-D dam-break case, an anti-roll tank of a vessel and the vertical motion of a fuel aircraft tank.

1.3 Structure of the Thesis

The thesis is structured as follows:

1. A general perspective of sloshing flows, physical phenomena involved and an overview of the numerical method to be employed have been discussed in **Chapter 1**.
2. Physical models and SPH numerical discretization are described in **Chapter 2**, including all the current formulations implemented in AQUAplusph, the code used in this PhD thesis.
3. **Chapter 3** deals with theoretical aspects of the method: boundary conditions are reviewed and a new methodology to compute the Shepard renormalization factor for the boundary integrals approach is proposed. Momentum and energy conservation aspects within the boundary integrals formulation are also studied.
4. A set of numerical tools and physical models that are implemented in AQUAplusph are presented in **Chapter 4**, validated with a set of benchmark test cases.
5. Finally, in **Chapter 5**, three sloshing applications are presented: a 3-D dam-break, an anti-roll tank, that is a naval industry relevant problem, and a vertical sloshing fuel aircraft tank.

Chapter 2

Theoretical background

This chapter describes the formulation used to model the physical problem, and the formalism used to describe it within the Weakly-Compressible-SPH (WC-SPH) framework.

2.1 Physical model

The governing equations for free-surface flows used in this work are the well-known Navier-Stokes equations. In a compressible general regime, assuming a barotropic fluid, they become in Lagrangian form:

$$\left\{ \begin{array}{l} \frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u}, \\ \frac{D\mathbf{u}}{Dt} = \mathbf{g} + \frac{\nabla \cdot \mathbb{T}}{\rho}, \\ p = p(\rho), \quad \mathbf{u} = \frac{d\mathbf{r}}{dt}. \end{array} \right. \quad (2.1)$$

Here, $\frac{D}{Dt}$ is the Lagrangian derivative, ρ is the fluid density, $\mathbf{g}$ a generic external volumetric force field and p the pressure, defined through a stiff Equation of State. The flow velocity, $\mathbf{u}$, is defined as the material derivative of a fluid particle position, $\mathbf{r}$.

The stress tensor of a Newtonian fluid, $\mathbb{T}$, is defined as [Gordillo Arias de Saavedra et al., 2017]:

$$\mathbb{T} = (-p + \lambda \text{tr}\mathbb{D})\mathbb{1} + 2\mu\mathbb{D}, \quad (2.2)$$

with $\mathbb{D}$ as the rate of strain tensor, i.e. $\mathbb{D} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$; $\mathbb{1}$ the identity matrix and μ and λ the viscosity coefficients.

2.1.1 Equation of State (EOS)

In order to close the system of Eqs. (2.1) in the weakly-compressible formalism, an Equation of State is needed to determine fluid pressure based on particle density. The compressibility is adjusted so that the speed of sound can be artificially lowered. This is necessary so that the time step can be maintained at a reasonable value. In [Monaghan, 2012] a set of different EOS were discussed, suggesting the following EOS as a suitable one for modeling free surface flows:

$$p = p_0 + b \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right], \quad (2.3)$$

where $\gamma = 7$ is the adiabatic constant, p_0 is the reference pressure and $b = c_s^2 \rho_0 / \gamma$ with ρ_0 being the reference density and $c_s = \sqrt{(\partial P / \partial \rho)|_{\rho_0}}$ the constant speed of sound.

Under the weakly-compressible assumption, a Taylor series around $\rho = \rho_0$ can be done. In practical applications, the linear term is sufficient to retain the properties of the EOS (see [Antuono et al., 2010]), leading to:

$$p = p_0 + c_s^2 (\rho - \rho_0), \quad (2.4)$$

which will be the expression used for all the cases presented all along this work.

To impose the weakly-compressible assumption, the sound speed is normally chosen such that $c_s = C v_{max}$ being v_{max} the maximum physical velocity within the problem and C a constant that sets the speed of sound to be at least ten times larger than the maximum fluid velocity ($C > 10$), keeping density variations to within less than 1%, and therefore not introducing major deviations from an incompressible approach. This stems from an order of magnitude analysis of the momentum equation, showing that the density variations are approximately proportional

to the square of Mach number Ma [Monaghan, 1994, Souto-Iglesias et al., 2006]

$$\frac{\Delta\rho}{\rho} \sim \left(\frac{v_{\max}}{c_s} \right)^2 = Ma^2. \quad (2.5)$$

2.2 Meshless method: SPH model

2.2.1 Continuous Model

SPH, despite initial focus on astrophysical problems, is currently extended to the simulation of the dynamics of general continuum media, such as solid mechanics and fluid flows.

The SPH method is based on an interpolation method that allows a field f , function of the spatial coordinates, to be expressed in terms of an integral interpolant evaluated at $\mathbf{x}$ over a generic domain Ω , such that:

$$\langle f(\mathbf{x}) \rangle = \int_{\Omega} f(\mathbf{y}) W(\mathbf{x} - \mathbf{y}, h) d\mathbf{y} \quad (2.6)$$

where $W(\mathbf{x} - \mathbf{y}, h)$ is known as the kernel function. A typical kernel shape is shown in Figure 2.1.

The kernel function acts as a “smoother” of the physical properties involved in the computation.

As it can be appreciated, kernel interpolants depend on two parameters, which are the two length scales which are intrinsic to SPH: the distance between points, $\mathbf{x} - \mathbf{y}$ (also $d\mathbf{r}$), and an interpolant or smoothing length, h . Kernel functions are normally decreasing functions that comply with a set of properties [Shadloo et al., 2016], which are established in (2.7), with s given and δ the Dirac delta function.

$$\left\{ \begin{array}{l} \int_{\Omega} W(\mathbf{x} - \mathbf{y}, h) d\mathbf{y} = 1, \\ \lim_{h \rightarrow 0} W(\mathbf{x} - \mathbf{y}, h) d\mathbf{y} = \delta(\mathbf{x} - \mathbf{y}). \\ W(\mathbf{x} - \mathbf{y}, h) = 0 \text{ when } |\mathbf{x} - \mathbf{y}| > s \cdot h \\ W(\mathbf{x} - \mathbf{y}, h) = W(\mathbf{y} - \mathbf{x}, h) \end{array} \right. \quad (2.7)$$

Any function that fulfills conditions in Eq. (2.7) could be used. Different examples of kernel functions are shown in Figure 2.2. For theoretical studies, the Gaussian function is the main option. However, since it is a function without compact support, it has been replaced for practical applications in the last decades by other options such as Spline [Monaghan and Lattanzio, 1985, Monaghan, 2005] and more recently Wendland kernels [Wendland, 1995]. Properties and differences between the different possibilities have been largely discussed by Dehnen and Aly [2012], showing as a result that Wendland functions are the most suitable for SPH practitioners. All along this thesis, a 5th degree class 2 Wendland kernel (WC2) will be used [Macia Lang et al., 2011], with compact support $s = 2$ unless otherwise specified. Therefore:

$$W(\mathbf{x}) = W_{C2}(\mathbf{x}/h) \frac{1}{h^d} = \beta \begin{cases} (2 - q)^4(1 + 2q), & \text{for } 0 \leq q \leq 2, \\ 0, & \text{for } q \geq 2, \end{cases} \quad (2.8)$$

where q is the normalized distance, defined as $|\mathbf{x}|/h$ and β is a constant that depends on the dimensionality of the problem. For 2-D simulations, $\beta = 7/64\pi$ and for 3-D simulations $\beta = 21/256\pi$.

Similarly to Eq. (2.6), the convolution can be applied to first order differential operators:

$$\langle \nabla f(\mathbf{x}) \rangle = \int_{\Omega} \nabla f(\mathbf{y}) W(\mathbf{x} - \mathbf{y}, h) d\mathbf{y}, \quad (2.9)$$

The problem here is that in general $\nabla f(\mathbf{y})$ is unknown. However, it is possible to use integration by parts to obtain a new expression such that:

$$\langle \nabla f(\mathbf{x}) \rangle = \int_{\Omega} f(\mathbf{x}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y} + \int_{\partial\Omega} f(\mathbf{y}) \mathbf{n} W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y}, \quad (2.10)$$

with $\mathbf{n}$ being the normal pointing outwards of the fluid domain at its boundary $\partial\Omega$. The symmetry property of the kernel (see Eq. 2.7) has also been applied. As it has been stated before, kernel vanishes outside of its kernel support, and therefore the second integral vanishes as well if the compact support is interior to the fluid domain Ω . If that is the case, the final

Figure 2.1: Typical shape of SPH kernel in 3-D and schematic view of a distribution of neighbor particles.

expression for a differential operator within the fluid is:

$$\langle \nabla f(\mathbf{x}) \rangle = \int_{\Omega} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y}. \quad (2.11)$$

When the kernel domain is truncated at a computational domain edge, the second term of Eq. (2.10) is no longer canceled out, and a different approach is needed.

2.2.2 Discrete SPH Model

The smoothed-particle hydrodynamics (SPH) method works by dividing the fluid into a set of discrete elements, referred to as particles. Therefore, the convolution presented in Eq. (2.6) of

Figure 2.2: Different types of kernel functions in 2-D used for SPH simulations.

an arbitrary field f for a generic i -th particle can be approximated at the discrete level as:

$$\langle f(\mathbf{r}_i) \rangle = \sum_j f_j W(\mathbf{r}_j - \mathbf{r}_i, h) V_j, \quad (2.12)$$

where V_j represents the volume of the particle j ($V_j = m_j/\rho_j$) and $\mathbf{r}_i$ denotes the position of the particle. The index j is used to denote all the particles inside the compact support of the kernel domain, the so-called neighbors (see Fig. 2.1).

Similarly, the spatial derivative of a quantity can be obtained easily by discretizing Eq. (2.9):

$$\langle \nabla f(\mathbf{r}_i) \rangle = \sum_j f_j \nabla W(\mathbf{r}_j - \mathbf{r}_i, h) V_j, \quad (2.13)$$

SPH formulation for the governing equations

Applying equations (2.12) and (2.13) to the Navier-Stokes equations in (2.1), we can get the expressions in discrete form. The SPH mass conservation equation reads:

$$\left\langle \frac{D\rho_i}{Dt} \right\rangle = \sum_j \rho_j (\mathbf{u}_j - \mathbf{u}_i) W(\mathbf{r}_j - \mathbf{r}_i) V_j. \quad (2.14)$$

where the velocity field has been appropriately defined so it vanishes if it is constant [Monaghan, 2005]. There are alternative formulations to obtain the density field, such as the summation formula [Español and Revenga, 2003], that computes density field from interpolation around neighbor particles.

$$\langle \rho_i \rangle = \sum_j m_j W(\mathbf{r}_j - \mathbf{r}_i). \quad (2.15)$$

Though mass conservation is assured, this alternative leads to wrong values of the density field near the free surface [Monaghan, 1992]. This is avoided with Eq. (2.14), and that is why it is used here.

Similarly, a linear momentum balance expression can be obtained:

$$\frac{D\mathbf{u}_i}{Dt} = -\frac{1}{\rho_i} \sum_j \mathcal{F}_{ij} + \mathbf{g}_i + \Gamma_i \quad (2.16)$$

where Γ_i corresponds to the viscosity term, that will be analyzed in the upcoming sections. Note here that, following the literature, the pressure gradient term $\mathcal{F}_{ij}$ can be discretized in several forms:

$$\mathcal{F}_{ij} = \begin{cases} (p_i + p_j) \nabla W(\mathbf{r}_j - \mathbf{r}_i) V_j, \\ \rho_i^2 \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla W(\mathbf{r}_j - \mathbf{r}_i) V_j, \\ (p_j - p_i) \nabla W(\mathbf{r}_j - \mathbf{r}_i) V_j \end{cases} \quad (2.17)$$

Top and middle approaches, following Bonet and Lok [1999] and Monaghan [1994] respectively, guarantee conservation of linear and angular momentum. The Monaghan [1994] term is known as the symmetric formulation, and is a common choice in SPH formulation. The drawback with

these two conservative formulations is that they fail in reproducing correctly the gradient of constant pressure fields when particles are arbitrarily scattered. Also, and more importantly, clumping of particles develops in areas where flow compression occurs, suggesting that repulsive forces between particles do not work properly in such regions, which is a phenomenon that is known as Tensile Instability [Colagrossi, 2005]. It will be shown later how this can affect simulation results in certain cases. In order to prevent Tensile Instability, last expression in Eq. 2.17 can be used at some controlled locations within the fluid domain, although losing conservation properties from the other formulations [Sun et al., 2018].

Viscosity

Viscous forces are deeply linked to the discretization of the Laplacian of the velocity field. The most straight-forward approach would be to apply the same procedure done for the first derivative operator. However, this option is not recommended as it has demonstrated to be poor in accuracy when particles start to disorder.

Alternatively, the Laplacian of the velocity has traditionally been treated as a combination of a finite differences scheme plus a smoothing process [Español and Revenga, 2003]. Two main approaches have been developed in this regard: the Morris et al. [1997] approach and the Monaghan and Gingold [1983] approach. The former reads:

$$\Pi_{ij} = 2\mu \sum_j \frac{(\mathbf{r}_j - \mathbf{r}_i) \cdot \nabla_i W_{ij}}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{u}_j - \mathbf{u}_i) V_j \quad (2.18)$$

The Morris term is inconsistent near the free surface if the boundary term is not computed along it [Cercos-Pita, 2015]. Alternatively, the Monaghan term takes the form:

$$\Pi_{ij} = \mu K \sum_j \frac{(\mathbf{u}_j - \mathbf{u}_i) \cdot (\mathbf{r}_j - \mathbf{r}_i)}{|\mathbf{r}_j - \mathbf{r}_i|^2} \nabla_i W_{ij} V_j, \quad (2.19)$$

where K is a spatial dimension parameter of the form $K = 2(d+2)$, with d being the dimension of the simulation (1-D, 2-D or 3-D)

SPH researchers are still attracted by the various formulations to approximate viscous terms

in SPH, as the solution is clearly not fully satisfactory. Some recent examples can be found in the works of Colagrossi et al. [2017], Zheng et al. [2018] or Bonet Avalos et al. [2020].

2.2.3 Artificial Diffusivity: δ -SPH

Numerical inconsistencies in the free surface (see e.g. Colagrossi et al. [2009]) led SPH practitioners to look for different alternatives to recover consistency near the free-surface. One of the first popular options was to apply a density Shepard renormalization after several time steps in order to smooth density field. Similarly, Ferrari et al. [2009] and Molteni and Colagrossi [2009] proposed different correction terms to the continuity equation that in order to recover zeroth order consistency.

Finally, a correction term to the continuity equation that recovered first order consistency near the free surface was born. This correction, called the δ -SPH model was first introduced by Antuono et al. [2010] and later revisited in Antuono et al. [2012].

It was initially devised to obtain smoother density fields and was modified to be consistent in the presence of a free surface. The scheme is characterized by the addition of a specific diffusive term inside the continuity equation that helps in reducing the spurious high-frequency noise that generally affects the density-pressure fields. In a similar fashion to the standard SPH, it conserves linear and angular momenta. Continuity equation written in (2.14) turns into:

$$\frac{D\rho_i}{Dt} = -\rho_i \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} V_j + \delta h c_0 \mathcal{D}_i, \quad (2.20)$$

with the diffusive term $\mathcal{D}_i$ given by:

$$\mathcal{D}_i = 2 \sum_j \psi_{ji} \frac{\mathbf{r}_{ji} \cdot \nabla_i W_{ij}}{\|\mathbf{r}_{ji}\|^2} V_j \quad (2.21)$$

with $\mathbf{r}_{ji} = (\mathbf{r}_j - \mathbf{r}_i)$ and

$$\psi_{ji} = \left\{ (\rho_j - \rho_i) - \frac{1}{2} (\langle \nabla \rho \rangle_j^L + \langle \nabla \rho \rangle_i^L) \cdot \mathbf{r}_{ji} \right\} \quad (2.22)$$

The symbol $\langle \nabla \rho \rangle_i^L$ indicates the renormalized density gradient (as it is presented in Randles and Libersky [1996]). As it was shown in Antuono et al. [2012], the parameter δ is not problem dependent, whilst its range of variation is quite narrow and only varies with $h/d\mathbf{r}$. Therefore, for a given value of $h/d\mathbf{r}$, there is no need for tuning it. In the present thesis, it has been set to 0.1 for all the simulations where it is used. Note that the δ -SPH method becomes the standard SPH method, presented in Eqs. (2.14) and (2.16) when δ is set to 0.

2.2.4 Integration scheme and time stepping.

An improved Euler integration (predictor-corrector) time scheme, is the option chosen for the time scheme, following the works of Souto-Iglesias et al. [2006] and Cercos-Pita [2015]. This is an explicit time integrator. Corresponding time evolution equations for the scheme proposed are shown here:

1. Predictor step

$$\begin{aligned}\mathbf{r}^* &= \mathbf{r}^n + \Delta t \mathbf{u}^n + \frac{(\Delta t)^2}{2} \left(\frac{d\mathbf{u}}{dt} \right)^n \\ \mathbf{u}^* &= \mathbf{u}^n + \Delta t \left(\frac{d\mathbf{u}}{dt} \right)^n \\ \rho^* &= \rho^n + \Delta t \left(\frac{d\rho}{dt} \right)^n\end{aligned}\tag{2.23}$$

2. Acceleration and density rate computations according to discrete equations from 2.1.

3. Corrector step

$$\begin{aligned}\mathbf{r}^{n+1} &= \mathbf{r}^* \\ \mathbf{v}^{n+1} &= \mathbf{u}^* + \frac{\Delta t}{2} \left(\left(\frac{d\mathbf{u}}{dt} \right)^* - \left(\frac{d\mathbf{u}}{dt} \right)^n \right) \\ \rho^{n+1} &= \rho^* + \frac{\Delta t}{2} \left(\left(\frac{d\rho}{dt} \right)^* - \left(\frac{d\rho}{dt} \right)^n \right)\end{aligned}\tag{2.24}$$

The time-stepping chosen in this work is only an option among a set of different possibilities, such as the Verlet or the Runge-Kutta schemes. Time step is chosen as the minimum over the following, taking as a reference different studies, such as Antuono et al. [2015] or Green [2016].

It is worth mentioning that the time stepping evolution algorithm chosen plays a role on the limit values of the CFL condition for the different time step limits.

$$\begin{aligned} \Delta t &\leq 0.44 \frac{h}{\delta c_s}, & \Delta t &\leq 0.125 \frac{h^2}{\nu}, \\ \Delta t &\leq 0.25 \min_i \sqrt{\frac{h}{\|\mathbf{a}_i\|}} & \Delta t &\leq \text{CFL} \min_i \left(\frac{h}{c_s + h \max_j |\pi_{ij}|} \right) \end{aligned} \quad (2.25)$$

with CFL being the Courant-Friedrichs-Levy condition factor for the propagation of pressure waves, ν the kinematic viscosity, a_i the acceleration of particle i and $|\pi_{ij}|$ defined as in Antuono et al. [2012]:

$$\pi_{ij} = \frac{(\mathbf{u}_j - \mathbf{u}_i) \cdot (\mathbf{r}_j - \mathbf{r}_i)}{|\mathbf{r}_j - \mathbf{r}_i|^2} \quad (2.26)$$

The CFL value for the Predictor-Corrector scheme is normally taken within the range [0.1 - 0.3] [Green, 2016], and taken as 0.2 in the present work.

Chapter 3

Theoretical aspects of the SPH method

Along this Chapter, theoretical aspects related to the SPH methodology to which this thesis has contributed will be discussed. In particular, linked to Grand Challenge 2 as described in **Chapter 1**, the problem of boundary conditions in SPH is presented in **Section 3.1**, and the different types of boundary conditions in a SPH context are described in **Section 3.2**. Following this presentation, **Section 3.3** focuses on existing boundary conditions approaches for wall modeling. Among the options available in the literature, boundary integrals are chosen as the methodology followed in this work. However, it is necessary to properly define the terms at the boundary in order to improve the stability of the solution. A new approach for wall modeling within the boundary integrals methodology, based on transforming the volume integral into a surface one and solving it semi-analytically, will be presented in **Section 3.4**.

After, in **Section 3.5** beneficial properties of fluid extension techniques are applied in a boundary integrals context, in order to derive aspects linked to moment and energy conservation, which are analyzed in **Section 3.6**. Some numerical examples will be assessed to assert validation of the new techniques in **Sections 3.4.4** and **3.7**.

3.1 The Problem of Boundary Conditions in SPH

Despite SPH originally developed in the context of astrophysics, in which domain boundaries do not play a significant role, new applications such as fluid dynamics problems, free-surface

flows or solid fracture strongly depend on boundary (BCs) and initial (ICs) conditions, which are used to close the equations that are needed for these models.

The intrinsic Lagrangian nature of the SPH method makes the procedure of including Boundary Conditions a challenge. Opposite to mesh based methods, in which actual domain edges can be specified, in SPH two main disadvantages stand out: on one hand the kernel support becomes incomplete, as there are no particles defined beyond the edges, leading to consistency problems and numerical errors. On the other hand, boundary conditions idea seems fictitious in a Lagrangian formalism in which interpolation points move along the simulation domain.

To include these boundaries in a SPH simulation, researchers use various techniques depending on the type of condition considered. These techniques can be classified in two main groups: fluid extensions and contour closure. The former consists on filling the compact support used in SPH near the boundary, where it lacks particles that allow for a correct particle interpolation. The latter relies on closing the contour with actual boundary segments – or particles, depending on the case, that contribute to the particle interpolation as a proper boundary. Both methods have advantages and shortcomings that will be discussed along this chapter.

This section is an attempt to summarize the most relevant references regarding boundary and initial conditions in the SPH fluid dynamics simulations context. The resulting list is obviously an open matter that is continuously evolving, as this topic is regarded as one of the key aspects for the SPH community, currently being one of the Grand Challenges established by the SPH SPHERic Group. However, currently there is not a complete review of all the publications regarding boundary conditions. It is thought that this is becoming a key task as several new methodologies arise every year, but boundary conditions approaches are only referred in some general SPH review papers [Monaghan, 2005, 2012, Gómez-Gesteira et al., 2010, Shadloo et al., 2016, Violeau and Rogers, 2016], or thesis [Green, 2016, Cercos-Pita, 2016].

Despite many advances have been done regarding SPH boundary conditions formulation, there are some key issues that remain to be addressed: on one hand, one of the main concerns is to see how it is possible to include BCs without losing the intrinsic SPH conservation properties, which is one of the main advantages of the method. Additionally, it is also important to develop boundary methods that are consistent. This issue has been addressed for some particular

aspects and formulations by different authors such as Macia Lang et al. [2011], who analyse the consistency of the no-slip boundary condition for different techniques or Souto-Iglesias et al. [2013], where a general perspective of consistency in the presence of boundaries is given while showing the equivalence of the Moving Particle Semi-implicit method (MPS) and the incompressible version of the SPH method (ISPH) .

On the other hand, regarding applicability, the principal effort is directed to include boundaries for real geometries. Regarding solid boundaries, 2-D and 3-D geometries might become greatly complex, and it is necessary to establish methodologies that are able to deal with corners, curved edges, etc. without increasing the computational cost dramatically [Bouscasse et al., 2013b]. Analogously, there is an extra effort to be done regarding inlet and outlet boundary conditions. Due to the Lagrangian nature of the method, inserting and removing particles in these areas needs to be carefully analyzed in order to achieve the requirements of the previous paragraph. Relevant references in this regard are Ferrand et al. [2017] or Vacondio et al. [2012b], among others.

Finally, regarding initial conditions, looking for a starting distribution of particles that avoids the onset of shocks once the time-integration starts becomes of capital importance. In this regard, works concerned on optimal particle distribution [Colagrossi et al., 2012] or damping at initial steps [Monaghan and Kajtar, 2009] have been developed.

Even though a general perspective of boundary conditions has been given, in the following sections a brief introduction to general types of boundary conditions will be presented, in order to introduce the main type of boundary condition when dealing with confined flows: wall boundary conditions.

3.2 Types of Boundary Conditions

As in any other CFD method, it is necessary to define both boundary conditions and initial conditions. The most relevant boundary conditions used for free surface flows are presented in this section.

3.2.1 Free surface boundary condition

Along the free surface, two boundary conditions must be satisfied: kinematic and dynamic boundary conditions. The kinematic boundary condition implies that material points located at the free surface must remain at the free surface during the evolution of the flow. This translates into:

$$u_n(\mathbf{x}) = \mathbf{u}(\mathbf{x}) \cdot \mathbf{n} = \mathbf{V}_n(\mathbf{x}) \quad \forall \mathbf{x} \in \partial\Omega_F \quad (3.1)$$

where $u_n(\mathbf{x})$ is the fluid velocity in the direction of the boundary normal at point $\mathbf{x}$ on the free surface Ω_F , and $\mathbf{V}_n(\mathbf{x})$ is the convective free surface velocity in that same direction.

The dynamic boundary condition is a consequence of the continuity of the stresses across the free surface. Assuming that surface tension is negligible, a free surface cannot stand neither normal stresses nor tangential shear stresses. This in practice means that the pressure is continuous across the interface and equal to the atmospheric pressure (p_a) at the free surface. In the case of a Newtonian fluid, this condition can be expressed as:

$$\mathbb{T} \cdot \mathbf{n}|_{FS} = (-p + \lambda \operatorname{tr} \mathbb{D}) \mathbf{n} + 2\mu \mathbb{D} \cdot \mathbf{n} = p_a \cdot \mathbf{n} \quad (3.2)$$

One of the greatest advantages of the SPH method comes from the fact that boundary conditions at the free-surface are satisfied intrinsically. An in-depth analysis of the role of free-surface in the SPH scheme is addressed in [Colagrossi et al., 2009], including a detailed description of the free-surface influence on the smoothed differential operators. The presence of a free surface has two main consequences: physical boundary conditions have to be satisfied on this surface and the interpolation accuracy has to be preserved close to the domain boundary. Indeed, when computing the SPH interpolation, some surface terms appear in both the pressure gradient and the velocity divergence terms. However, such terms are generally neglected by the SPH practitioners. Their deletion generally leads to pressure gradient formulas which do not converge to the right values near the free surface. Conversely, the widely used anti-symmetrized divergence operator converges even if the surface terms are not taken into account.

3.2.2 Inlet/Outlet boundary conditions

Inlet and outlet boundary conditions are intrinsically linked to open domains, with frequent application to the analysis of flows around floating or submerged bodies.

At the inlet, $\partial\Omega_I$ Dirichlet boundary conditions are normally considered for both the velocity and the pressure fields:

$$\begin{cases} \mathbf{u}(\mathbf{x}) = \mathbf{V}(\mathbf{x}), \\ p(\mathbf{x}) = P(\mathbf{x}), \end{cases} \quad \forall \mathbf{x} \in \partial\Omega_I. \quad (3.3)$$

Conversely, at the outlet, $\partial\Omega_O$, Neumann boundary conditions are usually imposed.

$$\begin{cases} \nabla \mathbf{u}(\mathbf{x}) \cdot \mathbf{n} = 0, \\ \nabla p(\mathbf{x}) \cdot \mathbf{n} = \mathbf{g} \cdot \mathbf{n}, \end{cases} \quad \forall \mathbf{x} \in \partial\Omega_O. \quad (3.4)$$

Currently, this topic has been addressed by various authors, that mainly base their different implementations on a buffer of particles located at the inlet and outlet domains, where particles can be added or deleted according to the flow evolution [Tafuni et al., 2018]. The topic has gained special attention in the last decade, and different implementations options can be found in the literature, such as Lastiwka et al. [2009], Federico et al. [2012], Vacondio et al. [2012b], Khorasanizade and Sousa [2016] and Tafuni et al. [2018].

Lately, Kassiotis et al. [2013] and Ferrand et al. [2017] adopt a different perspective, based on semi-analytic conditions to impose open boundary conditions.

Regardless the method employed, all of them should verify that mass conservation in time is assured, as this can turn into a critical aspect.

3.2.3 Solid boundary conditions

Other very important conditions to be satisfied in many engineering flows (both for internal confined flows and flows around bodies) are the boundary conditions at solid surface, $\partial\Omega_S$. Among them, the most important condition that solid boundaries must satisfy is the no-trespassing

condition, which reads:

$$\mathbf{u}_n(\mathbf{x}) = \mathbf{V}_n(\mathbf{x}), \quad \forall \mathbf{x} \in \partial\Omega_S. \quad (3.5)$$

where $\mathbf{u}_n(\mathbf{x})$ is the normal velocity of the fluid at the wall and $\mathbf{V}_n(\mathbf{x})$ is the normal velocity of the wall itself. For the tangential velocity, two options are possible: free-slip and no-slip conditions. The first implies that no restriction is imposed to the tangential velocity. Conversely, for the no-slip boundary condition the following must be satisfied:

$$\mathbf{u}_t(\mathbf{x}) = \mathbf{V}_t(\mathbf{x}), \quad \forall \mathbf{x} \in \partial\Omega_S. \quad (3.6)$$

where the sub-index t indicates the component of the vector contained in the tangential plane to $\partial\Omega_S$ in $\mathbf{x}$. The reader is asked to notice that the no-slip condition can be expressed in a more compact form such that:

$$\mathbf{u}(\mathbf{x}) = \mathbf{V}(\mathbf{x}), \quad \forall \mathbf{x} \in \partial\Omega_S, \quad (3.7)$$

as both normal and tangential velocities of fluid and wall are equal for particles at the wall. Regarding the pressure, the following boundary condition is considered:

$$\nabla p(\mathbf{x}) \cdot \mathbf{n} = \rho \left[\mathbf{g} - \frac{d\mathbf{V}(\mathbf{x})}{dt} + \nu \Delta \mathbf{u}(\mathbf{x}) \right] \cdot \mathbf{n} \quad \forall \mathbf{x} \in \partial\Omega_S \quad (3.8)$$

which is obtained by projecting the momentum equation on the solid boundary normal (see Bouscasse et al. [2013a]).

No trespassing condition - Elastic Bounce

Although a no-trespassing condition is imposed, sometimes it is necessary to reinforce this condition, ensuring that a particle cannot escape out of the domain edges. In those cases, the most common condition that is imposed is known as the elastic bounce. This technique consists on a force that is computed so that it prevents the particles from trespassing a wall [Simpson and Wood, 1996, Cercos-Pita, 2015]. Therefore, the normal component, $\mathbf{u}_{i_n}^*$, of particle i velocity,

$\mathbf{u}_i^*$, after the end of the time step corresponding to the boundary interaction is:

$$\mathbf{u}_{in}^* = \mathbf{u}_i^* \cdot \mathbf{n} = (\mathbf{V} - \mu_e \mathbf{u}_i) \cdot \mathbf{n}, \quad (3.9)$$

where μ_e is the elastic bounce factor. $\mu_e = 1$ corresponds to a full kinetic energy conservative interaction and $\mu_e = 0$ to a full kinetic energy dissipative interaction.

The main advantage of this condition relies on its simplicity and efficiency from the computational time point of view. It is also a very robust condition to satisfy the no-trespassing condition, able to deal with complex geometries and applicable in combination with any of the boundary techniques that have been developed. However, if it is used alone, its accuracy is low.

Apart from accuracy, the main inconvenience of the elastic bounce is that it breaks the natural momentum conservation of the SPH method. However, in cases when the flow is very energetic and mass is lost, as some particles escape the computational domain, these elastic bounce may be a reasonable trade-off between mass conservation and loss of accuracy.

3.3 Boundary Conditions in SPH

The SPH method is based on an interpolation inside a compact kernel support, this is, a finite volume around the interpolation point. When a fluid particle approaches a fluid domain boundary, only the particles located inside the intersection of the fluid domain and the kernel support are included in the SPH interpolants. Therefore, at a boundary this support is inexorably truncated (as it is shown in Figure 3.1). In the presence of a boundary, SPH operators do not cancel out any more as they are presented, and hence applying the same operators as in the bulk of the fluid will possibly lead to errors and unrealistic effects for the variables to solve. The different techniques used to account for these kernel truncation in the boundaries can be split into two main families, that can be seen in Figure 3.2: fluid extensions and contour closure.

Fluid extension methods aim to complete the kernel support following two main strategies: a

Figure 3.1: Schematic view of a point convolution in the presence of a boundary.

popular solution is known as the ghost particle technique and consists on mirroring particles with respect to the boundary. It was initially proposed by Randles and Libersky [1996] and later extended by others such as Colagrossi and Landrini [2003]. Ghost particle technique might be achieved by reflection across a boundary (as is the case for no-slip or free-slip boundary conditions) or by reflection in a set of particles fixed on the boundary [Ferrari et al., 2009]. An alternative to the ghost particle technique is known as the dummy particles method [Dalrymple and Knio, 2001], which is based on filling the kernel support by fixed particles that are initially distributed along the boundary. This methodology was later extended to the called Dynamic Particles technique [Crespo et al., 2007a]. Lately, dummy particles technique has been generalized in the fixed ghost particles technique, and several alternatives can be found in the literature, such as the ones proposed by Marrone et al. [2011] and Adami et al. [2012].

In contour closure methods, the volumetric contributions missing due to the truncated kernels are replaced by a surface contribution computed in the domain boundary. The oldest contour closure technique proposed is known as the Lennard-Jones boundary forces method. It was proposed by Monaghan [1994] and further developed by different authors, such as Monaghan and

Kajtar [2009]. In this methodology the boundary is discretized into points that exert repulsive forces on the surrounding particles. If contact forces are combined with kernel corrections that are included to account for incomplete kernel supports, a new methodology can be established, where additional terms in the volume integral that are non-zero in the presence of a boundary can be treated. This methodology was first described by Feldman and Bonet [2007] and later extended and named as the boundary integrals formulation by Ferrand et al. [2013], where the two mentioned approaches are combined by discretizing the boundary by points or vertices that represent a piece of area and reconstructing the kernel support by a renormalization.

Figure 3.2: Schematic view of the two main families when dealing with boundaries: fluid extensions (left) and contour closure techniques (right).

In conclusion, a definite method has not been found yet, having all of the proposed techniques advantages and drawbacks with respect to the other options. Boundary conditions in SPH methodology have therefore become a major point of interest. The different techniques developed by the SPH community in the last decades belonging to both families (fluid extensions and contour closure) will be now introduced to outline similarities and differences between them.

3.3.1 Kernel Corrections

A possible solution to the problem of boundary conditions in SPH is to let the kernel support become truncated and to replace it for a deformed or corrected version of itself, looking for recovering accuracy and consistency of the differential operators, though losing the momentum exact conservation properties [Vaughan et al., 2008]. This approach is actually not only confined to the cases in which a boundary term shows up, but in general is applied to provide a certain

order to the operators within a discrete set of particles.

Despite these inconveniences, the potential gain in accuracy and stability make them a potential and attractive option [Oger et al., 2007]. As an example, kernel corrections have been satisfactorily applied to improve consistency at the free surface [Colagrossi et al., 2009]. This is eventually an option that has been employed recursively in the literature of numerical methods, and especially in particle methods. Lately, kernel corrections are used in combination with other corrections to model solid boundaries, as is the case of the boundary integrals methodology, that will be discussed later on 3.3.4.

Different corrective terms have been available in the literature for a long time, such as the ones proposed by Belytschko et al. [1998], Bonet and Lok [1999], Vila [1999] or Chen and Beraun [2000].

In these techniques, the kernel function, $\nabla^n W(\mathbf{y} - \mathbf{x}, h)$ is replaced in Eqs. (2.9) and (2.11) by an alternative function $W_{\mathcal{L}}$, such that:

$$\nabla^n W_{\mathcal{L}}(\mathbf{y} - \mathbf{x}, h) = \mathcal{L}(\mathbf{x}) \nabla^n W(\mathbf{y} - \mathbf{x}, h), \quad (3.10)$$

and which guarantees certain properties of the interpolation at the discrete level for the $n - th$ derivative of the kernel.

In Belytschko et al. [1998], a careful analysis of several correction types is made, although such corrections have been already introduced by e.g. Liu et al. [1995], Johnson and Beissel [1996] or Randles and Libersky [1996]. It is mentioned there that the kernel corrections might be divided in two different types: those which correct the approximating functions, and those which correct the derivatives. For the former, a correction which allows for reproducing constants exactly is given by Shepard [1968]:

$$\mathcal{L} = \frac{1}{\gamma(\mathbf{x})} \mathcal{I}, \quad (3.11)$$

where $\gamma(\mathbf{x})$ is the Shepard renormalization factor, defined as:

$$\gamma(\mathbf{x}) = \int_{\Omega} W(\mathbf{y} - \mathbf{x}, h) dV. \quad (3.12)$$

The Shepard renormalization factor allows to recover the 0^{th} order consistency, remaining however inconsistent for the differential operators computation.

Conversely, a more complete correction for linear reproducing conditions that allows to recover 1^{st} order consistency corresponds to the Moving Least Squares (MLS) approximation, as it is proposed by Belytschko et al. [1994] and Randles and Libersky [1996]. The application of the MLS correction ensures that the gradient of any linear field is exactly evaluated.

Along this line, also Johnson and Beissel [1996] proposed such a correction of the derivatives of SPH for linear functions, by adjusting the standard smoothing functions for every node and every cycle, such that the derivatives are computed exactly for constant functions.

Chen and Beraun [2000] expanded the ideas introduced by Belytschko et al. [1998] and Randles and Libersky [1996], and presented a general method to solve non-linear dynamic problems. For the boundary terms, their approach was based on the same idea from Randles and Libersky [1996] and considered pseudo-ghost particles that are located half inside half outside the domain.

The deformed kernel is defined by a matrix of the form:

$$\mathcal{L}(\mathbf{x}) = \left[\int_{\Omega} (\mathbf{y} - \mathbf{x}) \otimes \nabla W(\mathbf{y} - \mathbf{x}, h) dV \right]^{-1}. \quad (3.13)$$

In Colagrossi et al. [2009], consistency and conservation features of such approach are analyzed. MLS kernel correction has been also widely applied for free surface boundary conditions when multiphase is not considered [Marrone et al., 2011, Bouscasse et al., 2013a].

Corrections to the interpolation of the functions and their derivatives can be jointly applied. For instance, Bonet and Lok [1999] proposed a mixed formulation in between these two ones, in which the fields are corrected by the Shepard function in Eq. (3.11) and the derivatives with the MLS correction in Eq. (3.13).

The kernel corrections have a set of drawbacks in a different context. For example, when a solid boundary is needed, no-trespassing condition cannot be guaranteed, as no boundary particles are inserted to define the domain.

To avoid this inconvenience, Kulasegaram et al. [2004] and later Feldman and Bonet [2007]

presented a combined technique in which a corrected kernel plus a boundary force term are derived from a variational formulation with the corrected operators at the boundaries. The main difference relies on the way the boundary contact force correction term γ (defined in Eq. (3.12)) and its derivative $\nabla\gamma$ are computed. The method is elegant, but becomes rather complex and computationally expensive for complex boundaries, such as in sharp corners or 3D geometries. These works were however the seed of the formulation that is known as boundary integrals, to be discussed in Section 3.3.4.

3.3.2 Boundary Forces

Nearly in parallel to the kernel correction technique, an alternative method was proposed, based on particles placed at the domain boundary, and first described by Monaghan [1994].

Boundary forces is a relatively simple methodology that can be applied in SPH when it is necessary to assure a no-trespassing condition on a solid wall. It consists of a set of dummy particles that are located along the boundary exerting a repulsion force over the fluid particles in the nearby.

Although it has shown to be a good methodology for wall-like boundary conditions, it is too simple due to its lack of consistency, just opposite to what happened in the kernel corrections methodology. However, the simplicity of this approach has resulted in a broad set of implementations. Different boundary forces based methodologies have been developed through the last decades. It can be considered that the most important methodologies are:

- **Repulsive particles:** This type of boundary technique is due to Monaghan [1994]. In this case the particles that lay on the boundary exert central forces on the fluid particles, in analogy with the forces among molecules. Thus, for a boundary particle and a fluid particle separated a distance r , the force per unit of mass has the form given by the Lennard-Jones potential. The Lennard-Jones force per unit mass reads:

$$f(\mathbf{r}) = D \left[\left(\frac{\mathbf{r}_0}{r_j - r_i} \right)^{p_1} - \left(\frac{\mathbf{r}_0}{r_j - r_i} \right)^{p_2} \right] \frac{(\mathbf{r}_j - \mathbf{r}_i)}{|\mathbf{r}_j - \mathbf{r}_i|^2} \quad (3.14)$$

that is set to zero if $\mathbf{r} > \mathbf{r}_0$, hence the force being only repulsive ($\mathbf{r}_0$ is the distance at which the force is zero). The constants p_1 and p_2 must satisfy that $p_1 > p_2$ and values are set to $p_1 = 12$ and $p_2 = 6$. Finally, the coefficient D is chosen depending on the physical configuration of the problem to be tested.

The Lennard-Jones potential was further analysed by Monaghan [1995]. The idea of associating a normal to the boundary particle is also found here for the first time in a SPH context. At that stage, fluid was prevented from penetrating the body, although disorder was found near the boundary. Reducing the spacing between boundary elements was thought as an option to help reducing the disorder, but it was unacceptable from the computational point of view at that point. Therefore, these radial forces produce a bumpy bottom with fluid particles bouncing over each boundary particle [Dalrymple and Knio, 2001].

Different aspects of this methodology, as well as different configurations, are analyzed by Cleary [1997, 1998], who tested the effect of various setup configurations and alternative boundary forces approaches. He found that boundary forces generate perturbations in the fluid particles if not treated properly, and looked for solutions to improve the stability and accuracy of this approach.

The method was refined by Monaghan [1995] and Monaghan and Kos [1999], by means of an interpolation process, minimizing the inter-spacing effect of the boundary particles on the repulsion force of the wall, smoothing it such that it is always acting normal to the boundary [Dalrymple and Knio, 2001]. Finally, the method proposed by Monaghan and Kos [1999] can be modified to adjust the magnitude of the force according to the local water depth and velocity of the water particle normal to the boundary. This modification was described in detail by Rogers and Dalrymple [2008], even though it can be a source of numerical instabilities in complex geometries.

This approach has been later used regularly. Some examples of the application of this methodology can be found in Monaghan et al. [2004], Monaghan [2006] and Monaghan and Kajtar [2009]. Additionally, in Souto-Iglesias et al. [2004] and Souto-Iglesias et al. [2006] another example of repulsive particles can be found. They use respectively an

elastic bounce technique (described in Section 3.2.3) and a derivation from the Lennard-Jones forces that were developed by Monaghan and Kos [1999]. This force is modified by deriving it from the gradient of the kernel, as it was already done by Gray and Monaghan [2003].

To sum up, in general, boundary force particles potential comes from the fact that they can be easily implemented. However, they generate normally more noise than other techniques and they involve a parameter that is problem dependent and needs to be set before simulations.

- **Dynamic particles:** These particles verify the same equations of continuity and of state as the fluid particles and are also included in the momentum equation. Therefore, an interesting advantage of these particles is their computational simplicity, as they can be calculated inside the same loops as fluid particles. However, they do not evolve but they remain fixed in position (fixed boundaries) or move according to some externally imposed function (moving objects like gates and wave-makers)

This approach arises as an alternative to the Lennard-Jones wall like boundary forces to overcome its drawbacks. In Dalrymple and Knio [2001], several rows of stationary particles are placed as boundaries in order to contain the fluid. Other examples of this methodology, in which they are used to study the interaction between waves and coastal structures can be found in Gómez-Gesteira and Dalrymple [2004], Gómez-Gesteira et al. [2005], Crespo et al. [2007b] and Crespo et al. [2008]. The model is further developed in Crespo et al. [2007a], where the method is described in detail.

The boundaries are found to behave elastically in the absence of viscosity. The boundary particles behave similarly to the repulsive particles approach, letting the fluid particles come near the edge up to a critical distance that depends on the energy of the incident particle. Indeed, the force exerted on a fluid particle i by a boundary particle j can be summarized as:

$$m_i \frac{du_i}{dt} = - \left(2c_s^2 \frac{W_{ij}}{(W_{ij} + W_0)^2} + m_i \Pi_{ij} \right) \nabla W_{ij} - \mathbf{g}, \quad (3.15)$$

which effectively depends on the sign of the gradient ∇W_{ij} , defined in the direction of the fluid particle, and $W_0 = W_{j=i} = W(\mathbf{r}_i - \mathbf{r}_i), h$ [Crespo, 2008].

The main drawback of this boundary technique arises in the early stages of the simulation, when the particles start moving. At that situation, particles start to separate from the walls and the density decreases locally, which generates a pressure decrease that results in a “pseudo-viscosity” forcing small groups of particles to remain stuck on the wall, producing a larger viscous effect on this area than the physical. Finally, as it happens with other techniques, there is not a guarantee that the fluid particles do not penetrate the boundary, this is, there is not an explicit trespassing condition imposed between the fluid particles and the boundary.

3.3.3 Fluid Extensions

A different alternative to complete the kernel support at the boundary is to add particles to fill in the gap with convolution points, hence virtually extending the fluid domain to this end. These particles, known as virtual or ghost particles, have to be added to the convolution integral.

The first task is to locate these particles in space - their number and positions. Regarding this aspect, three approaches have been used and documented in the literature. Some of these techniques are also displayed in Figure 3.3.

- **Mirrored (Ghost) Particles:** introduced by Randles and Libersky [1996], this is one of the first attempts to address the boundary conditions issue in SPH from a general perspective. Although other authors, such as Campbell [1989], Takeda et al. [1994] or Libersky and Petschek [1991] have introduced some aspects of the methodology to a limited extent, in Randles and Libersky [1996] a general view of a fluid extension methodology based on mirroring fluid field properties into a set of boundary particles is presented. To apply a boundary condition to a field value, the generated boundary particles have to carry the specified boundary value and the calculated values on the fluid particles. Hence, an interpolation is to be carried out between the boundary and the fluid values. Therefore,

Figure 3.3: Different examples of fluid extension techniques: on the left, Mirrored Particles; on the right, fixed particles.

the properties of the boundary particles, including their position, vary each time step. When a real particle is close to a contour (at a distance shorter than the kernel radius) then a virtual (ghost) particle is generated outside of the domain, constituting the mirror image of the incident one with respect to the boundary.

A slightly different approach was introduced by Ferrari et al. [2009], called the Virtual Boundary Particle Method (VBPM), that was later on further developed by Vacondio et al. [2012a] and Fourtakas et al. [2013]. The main difference between both formulations is the particle which is mirrored. In the Virtual Boundary Particle Method, it is the particle of interest to be computed that is mirrored with respect to the wall. Conversely, in the Virtual Ghost Particles technique the neighbors including the main particle are all mirrored.

Regarding the task of assigning field values to the new defined virtual particles, there exist different extension algorithms. The consistency of the different approaches has been reviewed by Macia et al. [2011] and Merino-Alonso et al. [2013].

The main benefits of ghost particles are that they are easy to implement and robust for relatively complex problems. On the other hand, there also exist some drawbacks in the application of this technique: some inconsistencies can be expected in the evaluation of the Laplacian, as reported by Macia et al. [2011]. Another inconvenience comes from the fact that the number of particles in the extended fluid is not previously known, making also

the memory required quite significant and heavily dependent on the geometry. Finally, applications for complex 3-D geometries with corners are not successful.

- **Fixed particles attached to the boundary:** in order to overcome some of the drawbacks derived from the mirrored ghost particles approach, in Marrone et al. [2011] a new approach is developed, called the fixed ghost particles (GP) approach. Conversely to the mirroring technique, in this approach a fixed layer of ghost particles is created at the boundary at the beginning of the simulation. To compute the quantities attributed to each ghost particle, an interpolation point is associated to it. This interpolation point is obtained by mirroring the position of the ghost particle into the fluid domain. At each time step, the ghost particles quantities are interpolated from there. To place the fixed ghost particles, the body boundary is assumed to be piece-wise regular and to be described by a spline discretized by body nodes. More details can be found in [Marrone et al., 2011] and [Bouscasse et al., 2013a]. The main advantage of using the fixed ghost particles instead of the standard ghost ones is that their distribution is always uniform and does not depend on the fluid particle positions. This allows for a simpler modeling of complex geometries.

The pressure, velocity and internal energy assigned to the fixed ghost particles, namely $(\mathbf{u}_s; p_s; e_s)$, are computed by using the values obtained at specific interpolation nodes internal to the fluid and uniquely associated with the fixed ghost particles [Bouscasse et al., 2013a]. Internal energy and pressure fields are mirrored on the fixed ghost particles to enforce a Neumann boundary condition. Alternative ways to compute pressure can be found in the literature. In Adami et al. [2012], a fixed ghost particles method is presented, in which a force balancing approach is used to obtain the pressure at the boundary. This approach ensures the no-trespassing condition and a smooth pressure field, and its implementation is relatively simple.

Regarding the velocity field, special treatment is needed. The ghost velocity depends on both the interpolated velocity $(\mathbf{u}^*)$ and the velocity on the boundary $(\mathbf{u}_b)$. In De Leffe et al. [2011] it is found that different mirroring techniques have to be used to evaluate $\langle \nabla \mathbf{u} \rangle$ and $\langle \nabla^2 \mathbf{u} \rangle$ to avoid inconsistencies and loss of accuracy. Differences between the

mirroring technique and the fixed particles technique are illustrated in Figure 3.3.

- **Templates of particles:** based on previous local virtual boundary particle methods (see e.g. Ferrari et al. [2009] or Vacondio et al. [2012a]), in Fourtakas et al. [2014] a novel 2-D and 3-D wall boundary treatment is described. It consists on generating a full stencil of virtual particles for each fluid particle at the beginning of the simulation, that moves accordingly with such particle. If a boundary is found during the movement at a distance below the kernel support, the corresponding associated particles are activated through a Ray casting algorithm. Surfaces are discretized through triangular planes.

To summarize, fluid extension techniques are a very robust methodology that has been applied in a wide range of cases. On the other hand, the main drawback of fluid extension methodologies is that for certain problems and geometries, either defining the virtual particles location or the corresponding field values becomes a difficult task.

3.3.4 Boundary Integrals

The last commonly used methodology in SPH to impose boundary conditions is known as the boundary integrals approach, which is actually a combination of two of the previous mentioned methodologies: kernel corrections and boundary forces. This methodology is based on the fact that the boundary term in the presence of a boundary (see Eq. (2.10)) should not be dropped, and integrated instead.

The first attempt to impose normal flux at a boundary corresponds to Campbell [1989]. Later, Kulasegaram et al. [2004] and Feldman and Bonet [2007] combine a corrected kernel and boundary contact forces, derived from variational principle with the corrected operators at the boundaries, naturally adding a surface term that is a consequence of the boundary terms not vanishing at the domain edge of the kernel support. Even though De Lefte et al. [2009] extended this idea to several types of boundaries, the first consistent boundary integral formulation was introduced by Macia et al. [2012] and Ferrand et al. [2013].

Ferrand et al. [2013] initially proposed a semi-analytic formulation in a WC-SPH framework. Later on, Cercos-Pita [2015] developed a purely numerical scheme. In both approaches, the

first order differential operator is defined as:

$$\langle \nabla f(\mathbf{x}) \rangle = \frac{1}{\gamma(\mathbf{x})} \left(\int_{\bar{\Omega}} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}; h) dV + \int_{\partial\bar{\Omega}} f(\mathbf{y}) \cdot \mathbf{n} W(\mathbf{y} - \mathbf{x}; h) dS \right) \quad (3.16)$$

This formulation shares indeed a lot of benefits of the boundary forces and kernel deformations, like the good capabilities to deal with complex geometries. Unfortunately, the main inconvenience comes from the fact that the Shepard renormalization factor, $\gamma(\mathbf{x})$, breaks the symmetry form of the operators, and therefore momentum conservation cannot be assured anymore. This is because, at the boundary, $\gamma(\mathbf{x}) \neq \gamma(\mathbf{y})$ when $\mathbf{x} \neq \mathbf{y}$. Additionally, in multiphase flows, the Shepard renormalization factor integral domain near the free surface boundary should consider all fluid domains in order to be consistent with boundary integrals formulation. However, it is common practice to only model the heavier phase, which is generally the most relevant. This reduces computational effort and has indeed become one of the greatest advantages of SPH for free surface flow simulations. On the other hand, the domain at the free surface is then incomplete, which causes a wrong computation of the Shepard renormalization factor. The only option for a correct procedure, as argued by Colagrossi et al. [2009], would be to explicitly model the lighter phase.

In the formulation proposed by Ferrand et al. [2013] the contour term is solved as a line integral that joins the solid wall element vertices. This methodology is further developed by Leroy et al. [2014] for ISPH in 2-D and later on extended to 3-D by Violeau et al. [2014] and Mayrhofer et al. [2015]. This formulation will be here renamed as the semi-analytic boundary integrals formulation (it is known as normal flux method in other contexts, as it is named in De Leffe et al. [2009]).

In parallel, following the same idea, in Cercos-Pita [2015] another methodology is developed, that solves the contour term numerically. This helps to easily extend the methodology to 3-D simulations, even though it assumes a truncation error. Despite the truncation error, vertex connectivity is avoided, hence helping in memory consumption efficiency aspects and keeping simplicity for boundary generation, as boundary elements can be assumed as square patches (particles with an associated area and normal).

Both formulations, then, are in principle able to deal with complex geometries.

3.4 A novel approach for the computation of the Shepard renormalization factor

In **Section 3.3**, boundary integrals methodology has been presented as the newest and potentially more powerful technique to deal with solid edges. It seems however necessary to further develop a broad set of aspects related to this methodology. In particular, it is important to improve the computation of the Shepard renormalization factor at the boundaries, in terms of accuracy, so shortcomings presented in Section 3.3 are, as much as possible, minimized. A novel formulation in this regard has been developed as part of this PhD thesis.

3.4.1 The role of the Shepard renormalization factor in the Boundary Integrals formulation

In Figure 3.1 a schematic view of a point convolution $\mathbf{x}$ in the presence of a boundary was shown. In such situation, the compact support of the kernel, $\Omega(\mathbf{x})$, can be divided into two different subdomains. The fluid subdomain is denoted by $\bar{\Omega}(\mathbf{x})$ and the subdomain outside the boundary, $\Omega^*(\mathbf{x})$. For the sake of simplicity, from now on, kernel function notation will be Ω , $\bar{\Omega}$ and Ω^* respectively, following the notation of Antuono et al. [2010].

Although fluid information in $\bar{\Omega}$ is always known, information beyond the wall (Ω^*) is not known *a priori* and hence different techniques, as the ones mentioned in Section 3.3, have been developed to account for this fact. Here, we will focus on the gradient operator, which plays an important role in SPH simulations. In the boundary integrals formulation, if the first order differential operator is expanded for a generic field f , considering both subdomains, and applying the divergence theorem, expression (3.16) is achieved.

In that expression, the Shepard renormalization factor $\gamma(\mathbf{x})$, as defined in (3.12), is introduced

to keep consistency. Here, the Shepard renormalization factor is recalled in discrete version:

$$\gamma(\mathbf{x}_i) = \sum_{j \in \text{Fluid}} W_h(\mathbf{x}_j - \mathbf{x}_i) V_j, \quad (3.17)$$

where $\mathbf{x}_i$ and $\mathbf{x}_j$ are the positions of a generic particle and one of its neighbors, respectively, and with V_j being particle j volume.

A set of advantages and drawbacks of this formulation in the continuum have been discussed in Section 3.3.4. An additional problem of the methodology expresses itself when the boundary integrals formulation moves on to the discrete level, i.e. when Eq. (3.17) is applied. In this context, even far from the boundary, $\gamma(\mathbf{x}_i) \neq \gamma(\mathbf{y}_j)$ when $\mathbf{x}_i \neq \mathbf{y}_j$, which may lead to values of the Shepard renormalization factor γ becoming greater than one. It might also happen that tensile instabilities appear because of the nature of the SPH interpolating kernels close to boundaries. Issues derived from these instabilities, such as sensitivity to particle disorder, clumping, or clustering clearly affect the computation of the Shepard factor, and might end up in unacceptable Shepard values and hence, instabilities leading to wrong simulations.

To overcome these disadvantages, a new boundary integrals formulation is here developed by defining a new integral at the boundaries that allows to transform the whole volume integral into a surface boundary integral.

3.4.2 Alternative geometrical formulation of the Shepard renormalization factor

A methodology to transform the volume integral to compute the Shepard renormalization factor (3.17) into a surface integral was first described by Feldman and Bonet [2007], extended later as a semi-analytical method for a generic 2-D profile in by Ferrand et al. [2013], Leroy et al. [2014] and finally incorporated by Violeau et al. [2014] to 3-D applications. However, these approaches can be unified as described in this Section.

Notice that the kernel is normalized, and we may integrate it by splitting its support as

$$\int_{\bar{\Omega}} W_h(\mathbf{y} - \mathbf{x}) d\mathbf{y} + \int_{\Omega^*} W_h(\mathbf{y} - \mathbf{x}) d\mathbf{y} = 1. \quad (3.18)$$

From the definition of the Shepard factor, Eq. (3.12):

$$\gamma(\mathbf{x}) + \int_{\Omega^*} W_h(\mathbf{y} - \mathbf{x}) d\mathbf{y} = 1. \quad (3.19)$$

The goal is to express the Shepard renormalization factor purely as a surface integral. In order to achieve that, a function $F(\mathbf{y} - \mathbf{x})$ is sought, such that

$$\int_{\Omega^*} \nabla \cdot [(\mathbf{y} - \mathbf{x}) F(\mathbf{y} - \mathbf{x})] = \int_{\Omega^*} W_h(\mathbf{y} - \mathbf{x}) d\mathbf{y}, \quad (3.20)$$

then, $\gamma(\mathbf{x})$ may be obtained from a boundary integral through the application of the divergence theorem:

$$\gamma(\mathbf{x}) = 1 + \int_{\partial\bar{\Omega}} \mathbf{n}(\mathbf{y}) \cdot (\mathbf{y} - \mathbf{x}) F(\mathbf{y} - \mathbf{x}) d\mathbf{y}. \quad (3.21)$$

The $\gamma(\mathbf{x})$ term may be therefore formulated in terms of surface integrals, which are purely geometrical, unlike volume integrals, which may change in time since the particles can move. They will also be clearly independent of any free surfaces that may appear, whilst volume integrals would be affected by the integration over an area with no particles.

Since the definition of Eq. (3.21) must apply for every integral, the general solution is given by the equality of the integrands. Moreover, as the kernel W_h depends only on $r := |\mathbf{y} - \mathbf{x}|$, the distance between $\mathbf{x}$ and $\mathbf{y}$, the function F can be sought so it also depends only on r , leading to

$$\frac{1}{r^{d-1}} \frac{d(r^d F(r))}{dr} = W_h(r), \quad (3.22)$$

where d is the dimensionality.

The solution to Eq. (3.22) depends, of course, on the choice of kernel. For the WC2 Wendland kernel [Wendland, 1995], and $s = 2$, expressions for $F(r)$ in reduced (non-dimensional) form

are given by:

$$F(r) = \frac{1}{h^d} \tilde{F}\left(\frac{r}{h}\right), \quad (3.23)$$

with $q := r/h$. In 2-D, $\tilde{F}$ takes the value:

$$\tilde{F}(q) = -\frac{7}{64\pi} \left[\frac{2}{7}q^5 - \frac{5}{2}q^4 + 8q^3 - 10q^2 + 8 \right] - \frac{1}{2\pi q^2}, \quad (3.24)$$

and in 3-D:

$$\tilde{F}(q) = -\frac{21}{256\pi} \left[\frac{1}{4}q^5 - \frac{15}{7}q^4 + \frac{20}{3}q^3 - 8q^2 + \frac{16}{13} \right] - \frac{1}{4\pi q^3}. \quad (3.25)$$

Both expressions in Eqs. (3.24) and (3.25) can in fact be separated into a polynomial part and a divergent part (as F is singular for $q = 0$), that will be denoted from now onwards $\tilde{F}_P$ and $\tilde{F}_D$ respectively. Therefore, in order to be consistent with the notation $F(r) = F_P(r) + F_D(r)$. This implies a set of constraints and a different treatment of the function F that will be discussed next.

3.4.3 Efficient evaluation of γ

The fact that the obtained function's $F(r)$ is singular for q going to zero, implies that one has to be careful when computing numerically the integral in Eq. (3.21), and this is especially relevant when approaching solid boundaries. Increasing the resolution might be a straight-forward approach to obtain a better approximation to integral in Eq. (3.21). However, even increasing above 50 times the fluid particle resolution does not render a substantial improvement while it results in an unacceptable increase of the computational cost, keeping in mind that a fast and reasonably accurate solution is being sought. To show it, Figure 3.4 illustrates how a resolution increase affects the Shepard renormalization factor $\gamma(\mathbf{x})$ compared to the theoretical solution for a fluid particle approaching a 90° corner along one of the boundaries, as it is depicted in Figure 3.5. The divergent term of the kernel has an influence on the last particle interpolation (the closest to the boundary), giving a wrong value of the Shepard renormalization factor which is independent of the resolution. The dashed line in Figure 3.4 represents the expected error derived from this last particle interpolation. As it can be appreciated, the error is nearly

Figure 3.4: Shepard value at the contour near a 90° corner for different kernel supports computed with $F(q)$ and compared to the analytical value. Dashed line is the black solid line displaced upwards $C = 0.021$, and represents the expected error. Horizontal axis: normalized distance q to the corner, vertical axis: Shepard value $\gamma(\mathbf{x})$.

constant and it follows $\gamma + C$, being in this case with a value of about $C = 0.021$. Since the value is the same for different resolutions, it can be guessed that the error follows the Shepard curvature.

Alternatively, Eq. (3.21) could be evaluated analytically. Such approach has been already considered by Violeau et al. [2014], leading however to involved expressions that, again, would be too costly from the computational point of view. Finally, another possibility, based on the previous one, would consist of solving once for multiple situations and tabulate the results. Unfortunately, a very high resolution would be needed again to obtain an accurate enough solution. It seems that none of these options are able to improve the solution. There is, however, another one, to be analyzed: Eq. (3.21) can be written as a summation on a number of patches, S_j :

$$\gamma(\mathbf{x}) = 1 + \sum_j \int_{S_j} \mathbf{n}(\mathbf{y}) \cdot (\mathbf{y} - \mathbf{x}) F(\mathbf{y} - \mathbf{x}) d\mathbf{y}. \quad (3.26)$$

If the curvature of the patches is neglected, they may be approximated by flat segments in 2-D

Figure 3.5: Fluid particle approaching horizontally a 90° corner. The elements in the dashed line represent the surface discretization for computing Eq. (3.21)

Figure 3.6: Discretization of the continuous boundary $\partial\bar{\Omega}$ (red line) to a set of discretized planar patches S_j (black line).

or flat panels in 3-D, so that normals are constant, as depicted in Figure 3.6. In this case,

$$\gamma(\mathbf{x}) - 1 \simeq \sum_j \mathbf{n}_j \cdot (\mathbf{y}_j - \mathbf{x}) \int_{S_j} F(\mathbf{y} - \mathbf{x}) d\mathbf{y}. \quad (3.27)$$

The expression $\mathbf{n}_j \cdot (\mathbf{y}_j - \mathbf{x})$, with $\mathbf{y}_j \in S_j$, is taken out of the integral since, for a flat patch, it equals r_j , the distance between $\mathbf{x}$ and the patch. The expression above is in fact similar to the ones proposed by Ferrand et al. [2013].

Finally, going back to Eqs. (3.24, 3.25), it has already been noticed that the kernel can be decomposed into a polynomial term, F_P , and a divergent term F_D . The integral of the polynomial term will still be solved numerically within the traditional boundary integrals formulation—either the semi-analytical [Ferrand et al., 2013] or the purely numerical [Cercos-Pita, 2015] one, whereas the divergent term is solved analytically. In Appendix A.1 it is shown that, based on the previous approximations, one can get in 2-D to:

$$\mathbf{n}_j \cdot (\mathbf{y}_j - \mathbf{x}) \int_{S_j} F_D(\mathbf{y} - \mathbf{x}) d\mathbf{y} = -\frac{1}{2\pi} \Delta\theta_j, \quad (3.28)$$

and in 3-D to:

$$\mathbf{n}_j \cdot (\mathbf{y}_j - \mathbf{x}) \int_{S_j} F_D(\mathbf{y} - \mathbf{x}) d\mathbf{y} = -\frac{1}{4\pi} \Delta\Omega_j. \quad (3.29)$$

In 2-D, $\Delta\theta_j$ is the angle subtended by segment S_j at point $\mathbf{x}$, which can be easily computed. Similarly, in 3-D $\Delta\Omega_j$ is the solid angle subtended by patch S_j at point $\mathbf{x}$.

The approach, as it is described by Mayrhofer et al. [2015], where Eq. (3.27) is directly addressed, yields a complex and costly formulation. That is partially solved by Violeau et al. [2014], where the same expression (3.27) is addressed, applying this time the Gauss' theorem to transform it in a line integral, which fits the semi-analytical formulation described by Ferrand et al. [2013], but has a poor performance in purely numerical approaches [Cercos-Pita, 2015]. In Appendix A.2 efficient ways to evaluate the subtended angle from Eqs. (3.28, 3.29), both in semi-analytical and purely numerical contexts, are described.

Incidentally, we may emphasize that different expressions to evaluate the subtended angle can be found, depending on the arbitrary discretization patch shape selected, in a similar fashion of mesh-based methods [Sozer et al., 2014]. In these algorithms it is assumed that the boundary is discretized in straight line segments for 2-D applications, while for 3-D applications different discretisations have been considered: triangles for the semi-analytical approach, and squares for the purely numerical one. Indeed, in the semi-analytical approach the computational

overhead of the connectivities is generally accepted, taking advantage of the well-known surface triangulation properties [Delaunay et al., 1934]. Conversely, in the purely numerical approach the boundary is discretized in square patches, as a natural 2-D extension of the volumetric discretization usually applied in SPH.

It is noteworthy that Eq. (3.28) in 2-D correctly predicts that for a point, $\mathbf{x}$, laying on one of the boundary patches,

$$\gamma(\mathbf{x}) - 1 \rightarrow -\frac{1}{2\pi}\pi = -\frac{1}{2}, \quad (3.30)$$

as long as only the patch containing $\mathbf{x}$ contributes to the summation (because all the others are either far away, or aligned with the patch). This is the expected result: $\gamma(\mathbf{x}) = 1/2$ close to a flat boundary. The same holds true in 3-D applying Eq. (3.29).

Therefore, if a point is detected at the contour, then it is just necessary to add $-\frac{1}{2}$ to the integration, such that the point itself will be ignored in the numerical integration. The accuracy

Figure 3.7: Shepard value for a fluid particle approaching a straight boundary. Black dashed line: monolithic expression from Eq. (3.24), red line: the same expression, but with the semi-analytic formulation as in Eq. (3.28), green line: analytical value of the Shepard renormalization factor.

in the evaluation of Eq. (3.27) has been tested and the results are shown in Figure 3.7, which shows the Shepard renormalization factor value for a fluid particle approaching a horizontal wall, from both the application of the monolithic expression of the new kernel ($F(q)$)—i.e. the straight-forward approach—, and from expressions (3.28) and (3.29)—in which the divergent part of the integral is solved analytically, as it is here proposed—. Both are seen to perform well far enough of the wall, whilst their behavior starts to differ when they are very close to the wall. Here is where the divergent part weights more and therefore, having an exact expression for this part makes the solution to be accurate near the wall. Otherwise, the increase in the particle resolution would need to be huge to diminish the error near the wall.

This derivation is extendable to any kind of planar boundary, including any angled corner. Figure 3.8 shows the results for a 90° corner. Performance is similar to the one shown in Figure 3.7, where a straight boundary is considered. In fact, results in Figure 3.8 (left) are equivalent to the test results shown in Figure 3.4. It can be appreciated that the correct value of $\gamma(\mathbf{x}) = 0.25$ is now reached at the corner when the divergent part of the kernel is integrated exactly with the new formulation. Additionally, several angled planar boundaries from different approaching

Figure 3.8: Shepard value for a 90° corner, for approaches along the vertical wall (left) and the diagonal (right). Legend as in Figure 3.7.

directions have been tested, as it is shown in Figures 3.9 and 3.10, giving satisfactory results regardless the combination, and proving that the formulation here presented is consistent. The new formulation is not only suitable for planar boundaries but for general boundaries indeed. Figure 3.11 represents the Shepard value at a circular boundary for a particle approaching radially from the center of the domain. Performance is seen to be similar to the previous tests

Figure 3.9: Shepard value for a 45° corner, for approaches along the vertical wall (left) and the diagonal (right). Legend as in Figure 3.7.

Figure 3.10: Shepard value for a 135° corner, for approaches along the vertical wall (left) and the diagonal (right). Legend as in Figure 3.7.

shown. The new formulation predicts correctly the value when approaching the boundary even having considered flat segments. Again, the monolithic formulation is not able to capture the correct value of the Shepard renormalization factor close to the boundary due to the effect of the singularity in $\tilde{F}_D$.

In order to assess the accuracy of the method as a function of the $h/(\Delta r)$ ratio, which controls the number of neighbors in an SPH calculation, we select the point closest to the corner of Figure 3.8 (the one with the worst results), and evaluate the relative error in the Shepard value, as this ratio is decreased. In Figure 3.12 the monolithic expression is seen to improve slightly as fewer neighbors are considered. Meanwhile, the semi-analytic method is seen to result in much lower errors. Both methods are affected by fluctuations as the number of neighbors becomes low. It is obvious that these are caused by the part that is common to both methods: the polynomial. Also, the monolithic part is well fit by the expression $\gamma + C$ with value for

Figure 3.11: Shepard value for a circular boundary for a particle approaching along the radius of the circle from the center to the boundary. Legend as in Figure 3.7

$C = 0.021$ as previously mentioned.

3.4.4 Application: 2-D Hydrostatic Tank

With the results shown in Section 3.4.3, it is expected that some current drawbacks of the boundary integrals formulation are avoided and results improve for any kind of geometry that is tested. In order to carry out a relevant test, a hydrostatic test case has been modeled with the open-source free tool AQUAplusph [Cercos-Pita, 2015], with both the standard and the new formulation.

A weakly-compressible δ -SPH model is solved. The δ -SPH scheme [Antuono et al., 2012, 2015, Cercos-Pita et al., 2016] introduced in 2.2.3 is considered in order to avoid numerical instabilities. The standard Navier-Stokes continuity and momentum equations for a barotropic fluid, as have been presented in Eqs. (2.1) are solved, including diffusive terms for both equations (see for instance [Antuono et al., 2012, Cercos-Pita et al., 2017]). A stiff linear equation of state, as in Antuono et al. [2010], Cercos-Pita et al. [2016] is used.

Figure 3.12: Relative error in the Shepard value at fixed point, close to a 90° corner as a function of $h/(\Delta r)$. Dashed line: monolithic expression; red line: approximation to the former; solid line: split expression.

The case consists of a tank set at rest for a certain period of time. The geometry is shown in Figure 3.13. The aim is to assess the performance of the new formulation introduced in previous section, to check whether the new boundary term computes the integrals accurately. This is a relatively simple test that nevertheless allows an easy assessment of the new formulation. In particular, eventual issues with the consistency of the operators, which may lead to spurious velocities and non-physical pressure values, and hence to the wrong computation of forces in the tank, can be detected.

Moreover, problems associated to particles leaving the boundary domain, which can occur with the standard formulation, are expected to be avoided. In addition to that, the traditional formulation makes it impossible to properly correct terms involving the divergence of the velocity, due to inconsistencies that arise in the presence of a free surface. This issue is now fixed, since with the new formulation the divergence of the velocity term is appropriately normalized with the Shepard factor term.

Figure 3.13: Geometry of the 2-D hydrostatic tank.

Density is set as $\rho = 998 \text{ kg/m}^3$ and dynamic viscosity μ as the standard value $\mu = 8.94 \times 10^{-4} \text{ Pa} \cdot \text{s}$ for water. There is therefore no artificial viscosity included in the simulation. Filling level is chosen as $H = 92 \text{ mm}$. Three different resolutions have been tested, with simulations with 10000, 50000 and 100000 particles. Also, different supports ($h/dr = 2, 3$ and 4) have been tried for the finest resolution. No boundary forces (i.e. elastic bounce) have been implemented to stop fluid particles from penetrating the solid walls.

Figure 3.14: Detail of the Shepard renormalization factor field at the right corner of the Hydrostatic 2-D tank set at rest for the traditional Shepard formulation (left) and the new Shepard geometrical formulation (right). Compact support $h/dr = 2$ and number of particles $N = 10000$. Reduced time is $t\sqrt{g/H} = 9.32$.

Figure 3.14 shows the tank at rest for the same simulation time, $t\sqrt{g/H} = 9.32$. Various aspects can be highlighted. The standard formulation of the Shepard renormalization factor leads to numerical errors in the interpolation. As it can be clearly appreciated, these errors make the particles at the free surface move, with some of them even jumping out of the tank. The simulation then turns unstable, even at early stages. Conversely, the novel formulation proposed computes the value of the Shepard renormalization factor exactly at the boundary, and therefore, particles remain without spurious movement and the simulation remains stable in time.

Besides these instability-related issues, close to the contact line, Shepard renormalization factor errors can be appreciated all along the free surface, when the original expression from Eq. (3.17) is considered. Furthermore, it can be appreciated that the original Shepard formulation is prone to produce wrong values, $\gamma(\mathbf{x}) > 1$, when tensile instabilities occur.

Figure 3.15: Evolution of the reduced kinetic energy for the hydrostatic case. Solid lines: new formulation for three different resolutions (10000, 50000 and 100000), dashed lines: traditional formulation.

In order to analyze the differences between both formulations more deeply, Figure 3.15 presents the kinetic energy evolution for three different resolutions. As it can be seen, in the standard formulation, the kinetic energy increases until the simulation fails. This time is shortened if the number of particles increases. Regarding the new formulation, the maximum value slightly increases as the number of particles increase, however its value is negligible and remains constant in time.

Figure 3.16: Evolution of the reduced L_2 hydrostatic pressure error for the hydrostatic case. Solid lines: new formulation for three different resolutions (10000, 50000 and 100000), dashed lines: traditional formulation.

Figure 3.17: Evolution of the non-dimensional L_2 hydrostatic pressure error for the hydrostatic case. Solid lines: new formulation for three different supports ($h/dr = 2, 3$ and 4), dashed lines: traditional formulation for the same supports.

Figures 3.16 and 3.17 show the error in the computation of the hydrostatic pressure according to the L_2 error of the pressure field (compared with the correct one), normalized by the exact hydrostatic pressure at the bottom of the tank. Figure 3.16 compares the traditional and the new formulations for three different resolutions, whilst Figure 3.17 represents the same two formulations for the biggest resolution and three different supports.

In Figure 3.16 results are seen to follow the same trends as for the kinetic energy with the traditional formulation. Errors in the pressure field start to rise until the simulation fails. The

failure occurs earlier for finer resolutions. Conversely, the new formulation has a relatively constant error that diminishes as the resolution increases, being almost the same for the two finer resolutions tested.

The same behavior is found when testing different supports (Figure 3.17). Whilst the traditional formulation tends to increase the error when support increases, in the new formulation this change is almost not noticeable, with a reasonable and constant error in time being obtained.

3.5 A link between Fluid Extensions and Boundary Integrals methodology through Local Surface Coordinates

In Section 3.3 the two main families of boundary approaches in SPH have been analysed, classifying them in methodologies based on the extension of the fluid domain beyond its boundaries and on kernel truncation by contour closure.

Regardless the methodology employed, all of them refer to different ways of solving the part of the truncated kernel where there is not information enough to complete the convolution. It is recalled here that this part has been referred to as Ω^* , defined as $\Omega^* = \Omega - \bar{\Omega}$ according to Figure 3.1. Indeed, the convolution of the differential operator of the generic field f within the kernel support Ω (presented in Eq. (2.11)) can be conveniently split into:

$$\int_{\Omega} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y} = \int_{\bar{\Omega}} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y} + \int_{\Omega^*} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y}. \quad (3.31)$$

In the expression above, boundary considerations are limited to the second integral in the RHS. Actually, this term is the contribution of fluid extension techniques on the overall integral, and it has been deeply analyzed in the literature (see e.g. Bouscasse et al. [2013a], Marrone et al. [2013], Cercos-Pita et al. [2017]). Conversely, boundary integrals approach what is taken into account is the fact that boundary terms does not vanish at the edge any more. Recalling Eq.

(3.16):

$$\langle \nabla f(\mathbf{x}) \rangle = \frac{1}{\gamma(\mathbf{x})} \left(\int_{\bar{\Omega}} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}; h) dV + \int_{\partial \bar{\Omega}} f(\mathbf{y}) \cdot \mathbf{n} W(\mathbf{y} - \mathbf{x}; h) dS \right), \quad (3.32)$$

A link between both approximations can be established, such that:

$$\begin{aligned} \int_{\Omega^*} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y} &\simeq \frac{1 - \gamma(\mathbf{x})}{\gamma(\mathbf{x})} \int_{\bar{\Omega}} f(\mathbf{y}) \nabla W(\mathbf{y} - \mathbf{x}, h) d\mathbf{y} \\ &+ \frac{1}{\gamma(\mathbf{x})} \int_{\partial \bar{\Omega}} f(\mathbf{y}) \mathbf{n} W(\mathbf{y} - \mathbf{x}, h) dS_{\mathbf{y}}. \end{aligned} \quad (3.33)$$

Expression above can be checked by substituting Eq. (3.33) into Eq. (3.31), which will lead to expression in Eq. (3.32).

Even though consistency for boundary integrals formulation has been analyzed in e.g. Macia et al. [2012], Ferrand et al. [2013], Leroy et al. [2016], Ferrand et al. [2017], as it is a relatively novel formulation, there are still open questions, such as consistency of second order differential operators. Additionally, momentum and energy conservation have been only superficially analyzed (see e.g. Cercos-Pita [2016]) showing that neither momentum nor energy conservation can be asserted within boundary integrals formulation.

In the following section, a novel approach in which beneficial properties of both methodologies are combined through Generalized Surface Local Coordinates is presented. The impact that this formulation has on conservation properties will be then thoroughly analyzed.

3.5.1 Generalized Surface Local Coordinates

As it has been already discussed, fluid extensions and boundary integrals formulations are linked by the relation in Eq. (3.33).

Analogously, a SPH volume integral —associated to fluid extensions— can be rewritten in the context of surface integrals, what will be called Surface Local Coordinates.

Let's start from the computation of the average value (that will be denoted by $\bar{F}$) in an arbitrary

volume, Ω , of an arbitrary field, f , as,

$$\bar{F}(\Omega) = \frac{1}{\Omega} \int_{\Omega} f(\mathbf{x}) dV(\mathbf{x}), \quad (3.34)$$

which vanishes identically at points at distance greater than d from the boundary $\partial\Omega$,

$$|\mathbf{y} - \mathbf{x}| > d, \forall \mathbf{x} \in \partial\Omega \implies f(\mathbf{y}) = 0. \quad (3.35)$$

At first glance, this may seem a very restrictive hypothesis, which limits the field of applicability. However, such fields are quite common in SPH modelling, for which $d = s \cdot h$, as d coincides with the radius of the support of the SPH kernel.

The aim is to express the volume integral in Eq. (3.34) as a surface integral through a transformation from Cartesian Coordinates to Local Coordinates (see Figure 3.18). Let's assume $\mathbf{x} \in \partial\Omega$ and approximate

$$\int_{\Omega} f(\mathbf{x}) dV \simeq \int_{\partial\Omega} \int_0^{s \cdot h} f(\mathbf{x} - \mathbf{n}(\mathbf{x}) \sigma) d\sigma dS(\mathbf{x}), \quad (3.36)$$

where $\mathbf{n}(\mathbf{x})$ is the outward pointing normal to the boundary at the surface point $\mathbf{x}$ and σ is the distance of the differential element to the boundary. Unfortunately, Eq. (3.36) cannot be easily discretized in a Lagrangian context, as it would require that interpolation points remained ordered along the normal, $\mathbf{n}(\mathbf{r}_i)$ of each generic i^{th} boundary element, regardless time instant. An alternative approach is necessary. The Dirac's Delta Sifting property can be applied to transform the line integral within Eq. (3.36) into a volume one [Onural, 2006], such that:

$$\int_0^{s \cdot h} f(\mathbf{x} - \mathbf{n}(\mathbf{x}) \sigma) d\sigma = \int_{\Omega(\mathbf{x})} f(\mathbf{y}) \delta((\mathbf{y} - \mathbf{x}) \cdot \mathbf{n}(\mathbf{x})) dV(\mathbf{y}), \quad (3.37)$$

where δ is the Dirac's Delta function. Applying the definition of δ in the continuum, in terms of the SPH kernel function, the following relation can be established:

$$\delta((\mathbf{y} - \mathbf{x}) \cdot \mathbf{n}(\mathbf{x})) = \lim_{h \rightarrow 0} W(\mathbf{y} - \mathbf{x}, h). \quad (3.38)$$

Figure 3.18: Schematic view of the integral along Local Coordinates.

Finally, the volume in the denominator of Eq. (3.34) can be expressed in a similar manner as it has been introduced in Section 3.4.2, according to the truncated domain under consideration:

$$\Omega = \int_{\partial\Omega(\mathbf{y})} W(\mathbf{z} - \mathbf{y}, h) dS(\mathbf{z}) \quad (3.39)$$

Combining Eqs. (3.34)-(3.38) the mean value of f can be found as:

$$\int_{\Omega} \bar{F}(\Omega) = \frac{1}{\Omega} f(\mathbf{x}) dV(\mathbf{x}) = \int_{\partial\Omega} \int_{\Omega(\mathbf{x})} \frac{f(\mathbf{y}) W(\mathbf{y} - \mathbf{x}; h)}{\int_{\partial\Omega(\mathbf{y})} W(\mathbf{z} - \mathbf{y}; h) dS(\mathbf{z})} dV(\mathbf{y}) dS(\mathbf{x}). \quad (3.40)$$

Eq. (3.40), hereinafter referenced as **Generalized Local Coordinates**, is therefore able to transform volume integrals to surface integrals, becoming indeed a bridge between fluid extensions and boundary integrals models. To this end, the line integral along the surface normal direction is replaced by an integral projection of the field at the boundary.

Eq. (3.40) is also valid at the discrete level, turning into:

$$\frac{1}{\Omega} \sum_{i \in \Omega} f(\mathbf{r}_i) V_i = \sum_{i \in \partial\Omega} \sum_{j \in \Omega(\mathbf{r}_i)} \frac{f(\mathbf{r}_j) W_{ij}}{\sum_{k \in \partial\Omega(\mathbf{r}_j)} W_{ij} S_k} V_j S_i. \quad (3.41)$$

The expression obtained has a potential range of valid applications. However, here it has been developed to study conservation properties in SPH. In particular, it will be used in the following section to compute forces within the boundary integrals formulation.

3.6 Conservation properties of the Boundary Integrals scheme

Conservation properties have always been a key aspect in the development of SPH and one of its most highlighted benefits. Momentum conservation has been analysed in general terms by several authors such as Bonet and Lok [1999], Vaughan et al. [2008], Owen [2014].

Energy conservation properties of the SPH method have been discussed by authors such as Randles and Libersky [1996], Bonet et al. [2004], Feldman and Bonet [2007], Antuono et al. [2015], Colagrossi et al. [2015], being however only a few authors who have addressed these problems in the presence of boundaries. For the fluid extensions methodology, fluid-solid energy interactions are analyzed by Cercos-Pita et al. [2017], whereas in the boundary integrals model, only a preliminary analysis has been carried out by Cercos-Pita [2016], showing that in the state of the art, neither momentum nor energy conservation are fully conserved.

In the present section, conservation of both momentum and energy will be analyzed within the boundary integrals methodology and the resulting expressions tested through a benchmark test case.

3.6.1 Conservative forces computation in Boundary Integrals formulation

It is a common practice in fluid dynamics to split the force exerted by the fluid on the boundary, $\mathbf{F}_{\Omega \rightarrow \partial\Omega}$, in the sum of the force due to the pressure and the force due to the viscous stresses. Indeed, by inspecting Navier-Stokes Eqs. (2.1), this division is clearly stated:

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega} = \mathbf{F}_{\Omega \rightarrow \partial\Omega}^p + \mathbf{F}_{\Omega \rightarrow \partial\Omega}^V, \quad (3.42)$$

with $\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p$ and $\mathbf{F}_{\Omega \rightarrow \partial\Omega}^V$ being the pressure and viscous force components respectively, and in which the bulk viscosity contribution is supposed to be zero.

Currently, the formulation of the viscous term in the boundary integrals methodology is still an open question [Macia et al., 2012]. Such question may be overcome by addressing the methodology to compute the pressure and the total forces, and subsequently obtaining the viscous component as the subtraction of the pressure component from the total force.

There are two features that usually play a chief role in the forces computation: momentum conservation and force per boundary subset. The former can be expressed as

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega} = -\mathbf{F}_{\partial\Omega \rightarrow \Omega}, \quad (3.43)$$

where $\mathbf{F}_{\partial\Omega \rightarrow \Omega}$ is the force exerted by the boundary on the fluid. The same expression can be considered for the pressure and viscous components. The latter consists on the possibility of splitting the boundary in an arbitrary number of subsets, computing the force exerted by the fluid on each one independently,

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega} = \mathbf{F}_{\Omega \rightarrow \partial\Omega_1} + \mathbf{F}_{\Omega \rightarrow \partial\Omega_2} + \cdots + \mathbf{F}_{\Omega \rightarrow \partial\Omega_n} \leftrightarrow \partial\Omega = \partial\Omega_1 \cup \partial\Omega_2 \cup \cdots \cup \partial\Omega_n. \quad (3.44)$$

In the next section, pressure forces computations will be analyzed following these premises, comparing the traditional approach with a novel approach that takes advantage of the Generalized Local Coordinates introduced in Section 3.5.1. Even though next section is dedicated mainly to the computation of pressure forces, similar approaches might be followed for the computation of viscous and total forces.

Pressure forces: traditional computation

The pressure force exerted by the fluid inside a closed domain can be computed as:

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p = \int_{\Omega} \nabla p(\mathbf{x}) dV(\mathbf{x}) \quad (3.45)$$

In the boundary integrals formulation, the pressure gradient is computed applying Eq. (3.16) to first expression in Eq. (2.17) (pressure gradient in symmetrized form), resulting into:

$$\begin{aligned} \langle \nabla p(\mathbf{x}) \rangle = \frac{1}{\gamma(\mathbf{x})} & \left(- \int_{\Omega(\mathbf{x})} (p(\mathbf{x}) + p(\mathbf{y})) \nabla W(\mathbf{y} - \mathbf{x}, h) dV(\mathbf{y}) \right. \\ & \left. + \int_{\partial\Omega(\mathbf{x})} (p(\mathbf{x}) + p(\mathbf{y})) \mathbf{n}(\mathbf{x}) W(\mathbf{y} - \mathbf{x}, h) dS(\mathbf{y}) \right) \end{aligned} \quad (3.46)$$

Eqs. (3.45) and (3.46) can be discretized to compute the total pressure force exerted on the boundary, obtaining a first expression such that:

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p \simeq \sum_{i \in \Omega} \langle \nabla p(\mathbf{r}_i) \rangle V_i, \quad (3.47)$$

where $\langle \nabla p(\mathbf{r}_i) \rangle$ denotes the SPH approximation of the pressure gradient in a boundary integrals framework,

$$\langle \nabla p(\mathbf{r}_i) \rangle = \frac{1}{\gamma_i} \left(- \sum_{j \in \Omega(\mathbf{r}_i)} (p_i + p_j) \nabla_i W_{ij} V_j + \sum_{j \in \partial\Omega(\mathbf{r}_i)} (p_i + p_j) \mathbf{n}_j W_{ij} S_j \right), \quad (3.48)$$

Eqs. (3.47) and (3.48) are therefore fulfilling condition (3.43), by definition, as they are the result of the direct application of momentum conservation definition. Unfortunately, such expression cannot be split in several boundary subsets, and therefore condition (3.44) is not satisfied. Hence, Eq. (3.47) cannot be used to compute the force exerted on a part of the boundary — see for instance Hadžić et al. [2005], Colicchio et al. [2006], Chen et al. [2007], Heller et al. [2009].

To overcome this issue, in Ferrand et al. [2013] it is already suggested an alternative forces computation formulation based on the application of the Divergence Theorem to Eq. (3.45),

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p = \int_{\partial\Omega} \langle p(\mathbf{x}) \rangle \mathbf{n}(\mathbf{x}) dS(\mathbf{x}). \quad (3.49)$$

Of course, Eq. (3.49) can be split into a sum of surface integrals on different bodies. The pressure $\langle p(\mathbf{x}) \rangle$ has to be extrapolated from the particles to the boundary. To this end, a

renormalized convolution can be used:

$$\langle p(\mathbf{x}) \rangle = \frac{1}{\gamma(\mathbf{x})} \int_{\Omega} p(\mathbf{y}) dV(\mathbf{y}) \quad (3.50)$$

Unfortunately, if Eqs. (3.49) and (3.50) are translated into discrete expressions, such that:

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p = \sum_{i \in \partial\Omega} \langle p(\mathbf{r}_i) \rangle \mathbf{n}_i S_i, \quad (3.51)$$

and

$$\langle p(\mathbf{r}_i) \rangle = \frac{1}{\gamma_i} \sum_{j \in \Omega(\mathbf{r}_i)} p_j W_{ij} V_j, \quad (3.52)$$

momentum conservation cannot be assured anymore, as it has been already drafted by Cercos-Pita [2016], hence becoming an unacceptable approach for a number of applications.

Pressure forces: Generalized Local Coordinates

Alternatively, Generalized Local Coordinates can be used instead. With the expression derived in Section 3.5.1, i.e. Eq. (3.40), Eq. (3.45) can be expressed in terms of a surface integral, such that momentum conservation is granted.

However, to apply this at the discrete level, i.e. Eq. (3.41) into (3.47), only fields vanishing far away from the boundary can be considered.

To this end, we can take of the following momentum conservation property of SPH (see e.g. Antuono et al. [2015]):

$$\int_{\Omega} \int_{\Omega(\mathbf{x})} (p(\mathbf{x}) + p(\mathbf{y})) \nabla_{\mathbf{x}} W(\mathbf{y} - \mathbf{x}, h) dV(\mathbf{y}) dV(\mathbf{x}) = 0, \quad (3.53)$$

which in the end means that interactions between fluid particles do not produce net moment,

and define a pressure gradient due to the boundary, combining Eqs. (3.40) and (3.45):

$$\begin{aligned} \nabla p^*(\mathbf{x}) := & -\frac{1-\gamma(\mathbf{x})}{\gamma(\mathbf{x})} \int_{\Omega(\mathbf{x})} (p(\mathbf{x}) + p(\mathbf{y})) \nabla_{\mathbf{x}} W(\mathbf{y} - \mathbf{x}, h) dV(\mathbf{y}) \\ & + \frac{1}{\gamma(\mathbf{x})} \int_{\partial\Omega(\mathbf{x})} (p(\mathbf{x}) + p(\mathbf{y})) \mathbf{n}(\mathbf{x}) W(\mathbf{y} - \mathbf{x}, h) dS(\mathbf{y}). \end{aligned} \quad (3.54)$$

Note that this expression is null far away from the boundary, and that the force expression is still valid,

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p = \int_{\Omega} \langle \nabla p(\mathbf{x}) \rangle^* V(\mathbf{x}). \quad (3.55)$$

Thus, Generalized Local Coordinates can be applied to Eq. (3.55), leading to an expression that in its discretized form reads:

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p = \sum_{i \in \partial\Omega} S_i \sum_{j \in \Omega_i} \frac{1}{\sum_{k \in \partial\Omega_j} W_{jk} S_k} \nabla p_j^* W_{ij} V_j, \quad (3.56)$$

with,

$$\begin{aligned} \nabla p_i^* = & -\frac{1-\gamma_i}{\gamma_i} \sum_{j \in \Omega_i} (p_i + p_j) \nabla_i W_{ij} V_j \\ & + \frac{1}{\gamma_i} \sum_{j \in \partial\Omega_i} (p_i + p_j) \mathbf{n}_j W_{ij} S_j \end{aligned} \quad (3.57)$$

The expression here obtained to compute the forces is valid provided that the Shepard renormalization factor is computed according to expression derived in this thesis, or any other alternative which grants that $\gamma_i = 1$ at any particle that is not affected by a solid boundary.

To sum up, Eq. (3.56) can be applied to compute pressure forces. Conservation properties of Eqs. (3.45) and (3.46) are kept, whilst the flexibility to compute forces on several bodies of Eqs. (3.51) and (3.52) is kept.

An analogous procedure can be followed to compute total force provided that:

$$\mathbf{F}_{\Omega \rightarrow \partial\Omega}^p = - \int_{\Omega} \rho(\mathbf{x}) \left(\left\langle \frac{d\mathbf{u}(\mathbf{x})}{dt} \right\rangle - \mathbf{g} \right) dV(\mathbf{x}). \quad (3.58)$$

3.6.2 Energy Conservation

In this Section, an analysis of the terms involved on the energy balance of the numerical fluid system is discussed. An analysis of this kind was carried out by Antuono et al. [2015] for isolated systems, and by Cercos-Pita [2016] for several boundary condition's approaches. However, the derivation of the energy balance equation for the boundary integral methodology remains undone. Hence, in this section the focus is on the analysis of the energy conservation properties of the boundary integral based SPH model in the presence of solid boundaries.

Energy Conservation equations at continuous level

The First Law of Thermodynamics, i.e. the conservation of energy, is stated as follows:

$$\frac{d\varepsilon_M}{dt} + \frac{d\varepsilon_I}{dt} = \mathcal{P}_{body/fluid}, \quad (3.59)$$

where ε_M and ε_I are respectively the mechanical and internal energies of the fluid, while $\mathcal{P}_{body/fluid}$ is the power delivered by the solid boundary $\partial\Omega$ to the fluid Ω .

The energy transfers due to volumetric forces deriving from a potential field are considered as a potential energy and included in the mechanical one. Heat conduction and radiation sources are not considered herein, neither power due to eventual interfaces with other fluids.

The power $\mathcal{P}_{body/fluid}$ is obtained by integrating the elementary power acting on each surface element of $\partial\Omega$, as discussed in Section 3.6.1. In that section, it was also shown that $F_{body/fluid}$ (and by extension $\mathcal{P}_{body/fluid}$) is normally split into two components, one associated to the pressure field and the other to the viscous forces. The former will be noted $\mathcal{P}_{body/fluid}^p$, whilst the latter will be denoted $\mathcal{P}_{body/fluid}^V$ from now onward. They are related to the forces through:

$$\begin{cases} \mathcal{P}_{body/fluid}^p &:= \int_{\partial\Omega_B} \mathbf{u}_B \cdot d\mathbf{F}^p, \\ \mathcal{P}_{body/fluid}^V &:= \int_{\partial\Omega_B} \mathbf{u}_B \cdot d\mathbf{F}^V, \end{cases} \quad (3.60)$$

with $d\mathbf{F}^p$ and $d\mathbf{F}^V$ being the elementary pressure and viscous forces of the body surfaces acting

on the fluid, $\partial\Omega_B$ is the solid boundary surface and $\mathbf{u}_B$ the velocity of the physical boundary.

Under the assumption of weakly-compressibility, the rate of change of internal energy ε_I is:

$$\frac{d\varepsilon_I}{dt} = \frac{d\varepsilon_C}{dt} - \mathcal{P}^V, \quad (3.61)$$

where $\mathcal{P}^V$ is the viscous dissipation rate of the fluid (which is always negative in the theoretical model, consistently with the Second Law of Thermodynamics), and ε_C is the elastic energy of the fluid due to the compressibility, i.e.:

$$\mathcal{P}^V = -2\mu \int_{\Omega} \mathbb{D} : \mathbb{D} dV, \quad (3.62)$$

$$\frac{d\varepsilon_C}{dt} = - \int_{\Omega} p \nabla \cdot \mathbf{u} dV = \int_{\Omega} \frac{p}{\rho} \frac{d\rho}{dt} dV. \quad (3.63)$$

Finally, the rate of change of mechanical energy can be expressed as the sum of the kinetic and potential energy contributions:

$$\frac{d\varepsilon_M}{dt} = \int_{\Omega} \rho \mathbf{u} \frac{d\mathbf{u}}{dt} dV - \int_{\Omega} \rho \mathbf{u} \cdot \mathbf{g} dV \quad (3.64)$$

Combining Eqs. (3.59) and (3.61), the First Law of Thermodynamics becomes:

$$\frac{d\varepsilon_M}{dt} + \frac{d\varepsilon_C}{dt} - \mathcal{P}^V = \mathcal{P}_{body/fluid}^p + \mathcal{P}_{body/fluid}^V \quad (3.65)$$

Analysis of energy conservation at the SPH level

The final aim is to assess if the RHS and LHS of Eq. (3.65) are equal at the discrete level. Let's start from Eq. (3.65), and analyze each of the terms involved in such expression derived in the previous Section. First, the mechanical energy variation rate $\frac{d\varepsilon_M}{dt}$ can be computed as the sum of the potential (ε_p) and the kinetic (ε_k) energy rates, leading to:

$$\frac{d\varepsilon_M}{dt} = \frac{d\varepsilon_p}{dt} + \frac{d\varepsilon_k}{dt} = \sum_{i \in Fluid} \rho_i V_i \mathbf{u}_i \left(-\mathbf{g} + \frac{d\mathbf{u}_i}{dt} \right) \quad (3.66)$$

where the acceleration term is affected by the boundary treatment approach that is used (from the ones presented in Section 3.3). In the present particular analysis, the expressions are the result of the application of the boundary integrals methodology. A similar approach has been followed for a ghost particle approach by Cercos-Pita et al. [2017].

Based on the definition of the acceleration term that was introduced in Eq. (2.16), deriving and rearranging, from the boundary integrals discretization perspective, in general one can write:

$$\begin{aligned} \frac{d\varepsilon_M}{dt} = & -\frac{1}{\gamma_i} \left(\sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j ((p_i + p_j) - \mu \pi_{ij}) \mathbf{u}_i \cdot \nabla_i W_{ij} \right. \\ & \left. + \sum_{i \in Fluid} \sum_{j \in BE} V_i ((p_i + p_j) - \mu \pi_{ij}) \mathbf{u}_i \mathbf{n}_j W_{ij} s_j \right). \end{aligned} \quad (3.67)$$

where *Fluid* account for the fluid particles and *BE* for the boundary elements. The first term in the RHS models the fluid contribution and the latter the influence of the boundary condition, and π_{ij} has been defined according to Eq. (2.26).

As it has been previously derived in Eq. (3.61), the rate of internal energy can be split into the rate of dissipated or irreversible energy, $\mathcal{P}_V$ (see Eq. (3.62)), and the rate of energy due to the compressibility or rate of elastic energy, ε_C , which is of the form:

$$\frac{d\varepsilon_C}{dt} = \sum_{i \in Fluid} V_i \frac{p_i}{\rho_i} \frac{d\rho_i}{dt}, \quad (3.68)$$

As it happened with the kinetic energy, the compressibility term $\frac{d\rho_i}{dt}$ is affected by the specific boundary condition approach used.

Taking into account the following relation (from Antuono et al. [2015]):

$$\sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j (p_i + p_j) \mathbf{u}_i \cdot \nabla_i W_{ij} = - \sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j p_i (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij}, \quad (3.69)$$

the elastic energy becomes, in the boundary integrals methodology, of the form:

$$\begin{aligned} \frac{d\varepsilon_C}{dt} = & \frac{1}{\gamma_i} \left(\sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j (p_i + p_j) \mathbf{u}_i \cdot \nabla_i W_{ij} \right. \\ & \left. - \sum_{i \in Fluid} \sum_{j \in BE} V_i p_i (\mathbf{u}_j - \mathbf{u}_i) \cdot \mathbf{n}_j W_{ij} s_j \right) \end{aligned} \quad (3.70)$$

Note that in Eq. (3.70) the Antuono relation from Eq. (3.69) is only applied to the fluid term, whilst the boundary term is left as in the original formulation.

The viscous dissipation rate $\mathcal{P}_V$, becomes (see Antuono et al. [2015] for details):

$$\mathcal{P}_V = -\frac{1}{2} \sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j \mu \pi_{ij} (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} \quad (3.71)$$

Finally, the fluid-solid exchange forces (i.e. the RHS of Eq. (3.59)) will be computed following the procedure explained in the previous Section, in order to conserve momentum. This means that pressure forces will be computed according to Eq. (3.56) and viscous forces as the remaining quantity between the total force in Eq. (3.58) and the pressure forces.

To sum up, terms corresponding to different components presented in Eq. (3.65), after rear-

ranging them, take the following form:

$$\left\{ \begin{array}{l} \frac{d\varepsilon_M}{dt} = -\frac{1}{\gamma_i} \left(\sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j ((p_i + p_j) - \mu \pi_{ij}) \mathbf{u}_i \cdot \nabla_i W_{ij} \right. \\ \quad \left. + \sum_{i \in Fluid} \sum_{j \in BE} V_i ((p_i + p_j) - \mu \pi_{ij}) \mathbf{u}_i \cdot \mathbf{n}_j W_{ij} s_j \right) \\ \frac{d\varepsilon_C}{dt} = \frac{1}{\gamma_i} \left(\sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j (p_i + p_j) \mathbf{u}_i \cdot \nabla_i W_{ij} \right. \\ \quad \left. + \sum_{i \in Fluid} \sum_{j \in BE} V_i p_i (\mathbf{u}_j - \mathbf{u}_i) \cdot \mathbf{n}_j W_{ij} s_j \right) \\ \mathcal{P}_V = -\frac{1}{2} \sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j \mu \pi_{ij} (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} \\ \mathcal{P}_{body/fluid}^p = \sum_{i \in \partial\Omega} \sum_{j \in \Omega(\mathbf{r}_i)} \frac{\langle \nabla p(\mathbf{r}_i) \rangle^* W_{ij}}{\sum_{k \in \partial\Omega(\mathbf{r}_j)} W_{ij} S_k} \mathbf{u}_B V_j S_i \\ \mathcal{P}_{body/fluid}^V = -\sum_{i \in \partial\Omega} \sum_{j \in \Omega(\mathbf{r}_i)} \rho_i \left\langle \frac{d\mathbf{u}(\mathbf{r}_i)}{dt} \right\rangle^* \frac{W_{ij}}{\sum_{k \in \partial\Omega(\mathbf{r}_j)} W_{ij} S_k} \mathbf{u}_B V_j S_i - \mathcal{P}_{body/fluid}^p \end{array} \right. \quad (3.72)$$

where all the terms have been previously defined. Eq. (3.59) can be rewritten as:

$$\frac{d\varepsilon_M^*}{dt} + \frac{d\varepsilon_C^*}{dt} - \mathcal{P}_V + (\mathcal{P}_s^V + \mathcal{P}_s^p + \mathcal{P}_s^C) = \mathcal{P}_{body/fluid}^p + \mathcal{P}_{body/fluid}^V \quad (3.73)$$

in which:

$$\begin{aligned} \frac{d\varepsilon_M^*}{dt} &= -\frac{1}{\gamma_i} \sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j ((p_i + p_j) - \mu \pi_{ij}) \mathbf{u}_i \cdot \nabla_i W_{ij} \\ \frac{d\varepsilon_C^*}{dt} &= \frac{1}{\gamma_i} \sum_{i \in Fluid} \sum_{j \in Fluid} V_i V_j (p_i + p_j) \mathbf{u}_i \cdot \nabla_i W_{ij} \\ \mathcal{P}_s^V &= \frac{1}{\gamma_i} \sum_{i \in Fluid} \sum_{j \in BE} V_i \mu \pi_{ij} \mathbf{u}_i \cdot \mathbf{n}_j W_{ij} s_j \\ \mathcal{P}_s^p &= -\frac{1}{\gamma_i} \sum_{i \in Fluid} \sum_{j \in BE} V_i (p_i + p_j) \mathbf{u}_i \cdot \mathbf{n}_j W_{ij} s_j \\ \mathcal{P}_s^C &= \frac{1}{\gamma_i} \sum_{i \in Fluid} \sum_{j \in BE} V_i p_i (\mathbf{u}_j - \mathbf{u}_i) \cdot \mathbf{n}_j W_{ij} s_j \end{aligned} \quad (3.74)$$

where:

- $\mathcal{P}_s^V$ represents the power transferred from the solid to the liquid particles through viscous diffusion.
- $\mathcal{P}_s^p$ is the power transferred from the solid to the liquid particles through pressure forces
- $\mathcal{P}_s^C$ is the power transferred from the solid to the liquid particles as a consequence of the compressibility of the fluid.
- $\frac{d\varepsilon_M^*}{dt}$ is the mechanical power **in the fluid**.
- $\frac{d\varepsilon_C^*}{dt}$ is the power in the fluid due to the compressibility **of the fluid**.

Finally, rearranging terms, having a distinction between terms coming purely from the fluid action, and the terms having an influence with the boundary, it can be written:

$$\frac{d\varepsilon_M^*}{dt} + \frac{d\varepsilon_C^*}{dt} - \mathcal{P}_V = \mathcal{P}_{body/fluid}^p + \mathcal{P}_{body/fluid}^V - (\mathcal{P}_s^V + \mathcal{P}_s^p + \mathcal{P}_s^C) \quad (3.75)$$

The aim is to check if Eq. (3.75) is truth for the boundary integral approach. For consistency, the overall term in the right hand side have to converge to zero in the limit $h \rightarrow 0$ and $\Delta x/h \rightarrow 0$, so that Eq. (3.65) is also true as the continuum is recovered in the SPH model.

3.7 Application test: moving square inside a box

To assess conservation properties that have been discussed in Sections 3.6.1 and 3.6.2, a test case is performed and results presented. It consists on an object fully submerged in a viscous fluid, subjected to a prescribed motion function, in the same fashion as the numerical test case performed by Cercos-Pita et al. [2017].

The geometry of the test case can be seen in Figure 3.19 (top). The object is a square of length L , and the outer domain is limited to $H = 5L$ and $B = 10L$. The object moves according to the time law presented in Figure 3.19 (bottom). The square experiences first an acceleration phase, until a constant velocity U is reached. This velocity is then maintained, whilst acceleration goes to zero. Reynolds number $Re = U D/\mu = 100$. Resolution is set as $L/\Delta x = 200$. Figure

Figure 3.19: Geometry and main parameters of the moving square test case (top) and motion law (bottom).

3.20 shows the evolution of the square at different time instants through the simulation. As it can be appreciated, flow detachment and wake are two visible aspects whose influence can be analyzed with this case.

Figure 3.21 presents pressure drag forces exerted by the fluid on the whole boundary, and the sum of forces computed by means of expression given in Eq. (3.58) for each of boundaries, i.e. the inner square $\partial\Omega_1$ and the outer box $\partial\Omega_2$. One of the advantages of the formulation

presented in this thesis for the computation of forces is that they can be computed on partial boundaries, such as in this case. Therefore, forces around the moving square can be calculated, avoiding complex treatment of external boundaries, such as in the work by Marrone et al. [2013], hence simplifying analysis.

In Figure 3.22 drag forces computed at the square boundary are compared with a Finite Difference Method solution. As it can be seen, there is a good correspondence between both solution at the stationary regime. On the other hand, the peak obtained with the SPH solution is over estimated when compared to the FDM solution.

Additional results for the pressure and viscous drag forces are presented in Figure 3.23. It can be seen that the main contribution to the total drag force is given by the pressure component. Both the SPH and the FDM solutions give similar results. However, there is a stronger discrepancy in the viscous forces register, even though quantitatively the difference is small and hence it has not a great impact on the total force. Further analysis will be needed to analyze these sources of discrepancy between both solutions. Also, a deeper analysis would be needed in order to quantify properly drag force at initial stages — i.e. the peak — similarly to what is performed in Marrone et al. [2013], but this is left for future analysis.

Figure 3.24 depicts time evolution of power terms corresponding to mechanical and elastic energy rate components, viscous dissipation and power due to forces on the moving square.

In Figure 3.25 time evolution of the different components in which fluid to boundary interactions are present are displayed. Even though pressure terms are practically equivalent, there is a stronger discrepancy in the viscous terms. This is somehow similar to what has been found in Cercos-Pita et al. [2017] for the ghost particles approach. In order to check whether this is due to an inconsistent formulation of the boundary integrals technique, in Figure 3.26 both the pressure and viscous difference between both terms depicted in Figure 3.25 is shown. For both the pressure and viscous terms, the difference between both terms decreases as resolution increases, tending apparently to zero for a greater number of particles. Even though these results should be treated carefully, as it seems that pressure term consistency reaches a limit for $D/\Delta x > 100$, differences are considerably close to zero. Additionally, in the viscous term this evolution towards zero is clearly appreciated even for the finest resolution.

Despite the fact that further analysis would be needed, promising results have shown the potential of the current formulation for the computation of forces, as it is a conservative formulation that, additionally, is consistent from an energetic point of view.

Figure 3.20: Evolution of the square moving inside a box case at three different time instants. Figures are colored with velocity field magnitude values.

Figure 3.21: Drag coefficient for global forces computed by two different means: black line corresponds to total force exerted by the fluid on the whole boundary, whilst red line to the sum of partial forces computed on each of the boundaries, $\partial\Omega_1$ and $\partial\Omega_2$.

Figure 3.22: Drag force at $Re = 100$ predicted by SPH (black solid line) and Finite Difference Method (red line) for a moving square.

Figure 3.23: Pressure (left) and viscous (right) components of the drag force of a moving square at $Re = 100$. Black line corresponds to forces predicted by SPH, whilst red line to a Finite Difference Method solution.

Figure 3.24: Time evolution of diverse power components of a moving square at $Re = 100$.

Figure 3.25: Time evolution of power components related to fluid-solid interactions: top plot represents pressure terms, whilst bottom plot represent viscous terms. Moving square at $Re = 100$.

Figure 3.26: Moving square at $Re = 100$: left figure represents the differences between pressure ($\mathcal{P}_{body/fluid}^p - \mathcal{P}_s^p$) and right figure to the differences between viscous ($\mathcal{P}_{body/fluid}^V - \mathcal{P}_s^V$) force terms computed from the fluid and from the boundary perspectives.

Chapter 4

Implementations

In order to improve the understanding of the physical phenomena involved in the simulation of sloshing flows, a set of capabilities have been added to the SPH code used, AQUA_{gpusph}.

A description of AQUA_{gpusph} will be given first, discussing the capabilities that are already implemented, as well as the structure of the code.

Two tools that are relevant for the study of free surface flows have been implemented within the boundary integrals methodology: a particle packing algorithm and a free surface detection algorithm. Implementation details and relevant results for each of these will be given.

Additionally, two different physical models have been included in AQUA_{gpusph}, adapting them to the boundary integrals approach: a LES-model and a phase change model. The models are also discussed and results for benchmark cases are shown.

4.1 AQUA_{gpusph}

AQUA_{gpusph} (Another Quality GPU-accelerated SPH) is a fully free and open software developed by Cercos-Pita [2016]. It is currently licensed under the GPLv3 terms, thus implying that the users are welcome to read, edit and redistribute the code, with the main limitation that the redistributed versions must be shared with the same license. Of course, the possibility of accessing the source code of the program, as well as the source code of the tools packaged

within it, is not only a desirable feature for the software in general, but also a mandatory one if the research community is the main target.

Basic information that will be necessary to understand implementations will be recalled here. For additional information, the readers are referred to Cercos-Pita [2016] and other resources such as Cercos-Pita [2013, 2015]. Latest improvements in which novel capabilities are added can be found in Cercos-Pita and Duque [2019]

AQUA_{Agpusph} main advantages are its modularity, flexibility and fully free packages. All these characteristics make AQUA_{Agpusph} a very attractive tool for researchers.

One of the aims of AQUA_{Agpusph} developers is to provide a fully free software to the community, able to run in multiple platforms, meaning thus a step forward compared to other open-source softwares. As many other SPH codes, AQUA_{Agpusph} is GPU accelerated. The main difference with the other tools is that this is achieved with an OpenCL architecture, instead of the proprietary framework CUDA. This way the user is not restricted to a unique vendor. Therefore, the usage of OpenCL pushes for the freedom and flexibility of the code.

Being flexible also means that it allows for the implementation of new features easily. As SPH is an evolving method that brings up new methodologies every year, it is important to have a tool that permits implementing different methodologies simply, combining them to the benefit of the user. AQUA_{Agpusph} is divided into three different levels or modules (see Figure 4.1, where this level division is schematically depicted). The main reason behind such segmentation is that the user avoids to deal with a complex programming language when trying to implement new methodologies. Hence the lowest level corresponds to the core of AQUA_{Agpusph}, where the most complex pieces of code are located. Under normal circumstances, the user will not need to modify or even recompile this piece of code. The pieces of code that the user will modify are located at the top level, and are composed mainly by OpenCL and Python scripts. The connection between both levels is done through an intermediate level where XML files are located. The main purpose of these files is to compose modules (which are also called presets) of code generated at the user level to be loaded and executed by the lower level.

Therefore, the user will mainly interact with the code by generating presets. These include

Figure 4.1: Sketch of AQUAgpusph modular distribution in levels: top corresponds to lower level and bottom to user level.

different sets: variables, tools and reports. An example including all these can be seen in Figure 4.2.

Variables are the values that users employ to input and output from the tools. Mainly, they can be divided into two groups: scalars, vectors and arrays. The former are single-value variables that can be easily handled in read-write operations. Vectors are a group of N scalars, being N an integer from 1 to 4. The latter are fixed-length lists of scalars or vectors that are mainly used to loop over them within the openCL tools. In this context, they are noted with a $*$ identifier. A comprehensive list for the different groups can be found in Table 4.1 (taken from Cercos-Pita [2016]).

```

1 <sphInput>
2
3 <Variables>
4   <!--Kinetic energy rate-->
5   <Variable name="dekdt" type="float*" length="N" />
6   <Variable name="dEkdt" type="float" value="0.0" />
7 </Variables>
8
9 <Tools>
10  <Tool action="insert" after="cfd interactions,cfd lap p" name="cfd fluid power"
      entry_point="fluid" path="{@ROOT_PATH}/resources/Scripts/cfd/Energy/Power.cl" type="
      kernel"/>
11  <Tool action="insert" after="cfd power" type="reduction" name="cfd dEkindt" in="dekdt"
      out="dEkdt" null="0.f">
12    c = a + b;
13  </Tool>
14 </Tools>
15
16 <Reports>
17  <Report type="screen" name="Energy" fields="dEkdt;" color="blue" bold="false"/>
18  <Report type="file" name="Energy file" fields="t,dt, dEkdt" path="Power.dat"/>
19 </Reports>
20
21 </sphInput>

```

Figure 4.2: Example of an XML intermediate file, including the definition of variables, tools and reports.

The tools are the elements executed at each time step that perform operations and build the iteration loop. There exist four types of tools:

- **OpenCL tools:** divided in pieces of code (namely kernels), each of them carrying out a set of operations involving variables.
- **Python scripts:** pieces of code built in Python, normally to perform preprocessing (Particle generation) or post-processing (plot or data manipulation) actions.
- **Dummy tools:** present to indicate an event to other modules.
- **muParser tools:** perform operations such as a summation over particles, etc.

Finally, reports are pieces of code used to give information to the user. They can be printed through the screen or stored in files that can be used later for plotting or manipulation.

In its last version (AQUA_{Agpusph}-3.0), a fully working Weakly Compressible SPH code is delivered, including a set of tools and methodologies that are already implemented and at a disposal

Table 4.1: List of variables available in AQUAopusph

Variable	Type	Description
int	Scalar	Integer scalar variable
unsigned int	Scalar	Unsigned integer scalar variable
float	Scalar	Floating point scalar variable
ivecN	Vector	Vector of N integer components. It will take the form ivec2 for 2-D simulations and ivec4 for 3-D simulations
uivecN	Vector	Vector of N unsigned integer components. It will take the form uivec2 for 2-D simulations and uivec4 for 3-D simulations
vecN	Vector	Vector of N floating point components. It will take the form vec2 for 2-D simulations and vec4 for 3-D simulations
int*	Array	Array of integers
unsigned int*	Array	Array of unsigned integers
float*	Array	Array of floating point values
ivecN*	Array	Array of vectors of N integers components. Called ivec2* for 2-D simulations and ivec4* for 3-D simulations
uivecN*	Array	Array of vectors of N unsigned integer components. Called uivec2* for 2-D simulations and uivec4* for 3-D simulations
vecN*	Array	Array of vectors of N floating point components. Called vec2* for 2-D simulations and vec4* for 3-D simulations
matrix*	Array	Array of floating point matrices. 2x2 matrix in 2-D (4 elements each) and 4x4 matrix in 3-D (16 elements each).

for the practitioner to be used. Among others, they include:

1. δ -SPH methodology introduced by Antuono et al. [2010], with corrections done by Fatehi and Manzari [2011]. Actually, the latter is the formulation implemented here.
2. Both physical and artificial viscosity, including Laplacian formulations by Morris et al. [1997] and Monaghan and Gingold [1983].
3. Multi-resolution features, including particle split and coalesce [Vacondio et al., 2013] and variable resolution [Zisis et al., 2016].
4. A wide range of boundary conditions, including: boundary integrals [Ferrand et al., 2013, Cercos-Pita, 2015], fixed ghost particles [Bouscasse et al., 2013b], elastic bounce [Cercos-Pita, 2015], inflow/outflow [Federico et al., 2012].
5. 6-DOF motion for rigid bodies.
6. MLS correction by Randles and Libersky [1996].
7. Energy and force computation for post-processing and analysis [Cercos-Pita et al., 2017].
8. Predictor-Corrector scheme for time integration [Souto-Iglesias et al., 2006].

All along the Chapter, several examples on how the tools can be used on novel methodologies will be shown, followed by results derived from such implementations.

4.2 Particle packing algorithm

In SPH, the initial distribution of particles plays an important role, as spurious motions might be induced at initial stages, affecting considerably the flow evolution. In Colagrossi et al. [2012] an analysis of the influence of initial distribution of particles was carried out. As a result, an algorithm to set an initial “equilibrium” distribution of particles was presented for the fixed ghost particle approach. Here, the same algorithm is replicated, extending it also to a more

general framework that includes a contour closure technique such as boundary integrals. Results obtained from both approaches for the same test case are compared for different resolutions.

The starting point of the analysis comes from the comparison of Navier-Stokes equations at continuous and discrete levels. A noticeable difference arises from the satisfaction of the kernel properties (see Eq. (2.7)), which are exact in the continuum, at the discrete level. One of the reasons is the local unevenness of particle distribution. Let's define two new variables in this context:

$$\begin{cases} \Gamma(\mathbf{x}) = \int_{\Omega} W_{ij} d\mathbf{y} \\ \nabla\Gamma(\mathbf{x}) = \int_{\Omega} \nabla_i W_{ij} d\mathbf{y} \end{cases} \quad (4.1)$$

These new variables $\Gamma(\mathbf{x})$ and $\nabla\Gamma(\mathbf{x})$ can be regarded as a quantification of the irregularity in the particles' distribution. For avoiding spurious movement at static conditions, particles' distribution must achieve (turning now into the corresponding version at the discrete level) $\Gamma_i = 1$ and $\nabla\Gamma_i = 0$.

This aspect is specially relevant in the presence of a solid edge. Indeed, near the boundaries, both variables need to be defined appropriately. Therefore, Eqs. (4.1) turn into:

$$\begin{cases} \Gamma_i = \sum_{j \in Fluid} W_{ij} V_j + \sum_{j \in BE} W_{ij} V_j = \sum_{j \in Fluid \cup BE} W_{ij} V_j \\ \nabla\Gamma_i = \sum_{j \in Fluid} \nabla_i W_{ij} V_j + \sum_{j \in BE} \nabla_i W_{ij} V_j = \sum_{j \in Fluid \cup BE} \nabla_i W_{ij} V_j \end{cases} \quad (4.2)$$

for the ghost particles technique and into:

$$\begin{cases} \Gamma_i = \frac{1}{\gamma_i} \sum_{j \in Fluid} W_{ij} V_j \\ \nabla\Gamma_i = \frac{1}{\gamma_i} \left(\sum_{j \in Fluid} \nabla_i W_{ij} V_j + \sum_{j \in BE} W_{ij} \cdot \mathbf{n}_j S_j \right) \end{cases} \quad (4.3)$$

for the boundary integrals methodology.

Following definition of Γ and $\nabla\Gamma$ in Eq. (4.1) and after rearrangement of terms, the operators

in Euler equations can be rewritten in terms of the novel variables as (for a full derivation of the following expressions, see Colagrossi et al. [2012]):

$$\begin{cases} \langle \nabla \cdot \mathbf{u} \rangle_i &= \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} V_j = \Gamma_i (\nabla \cdot \mathbf{u})_i + \mathcal{O}(h), \\ \langle \nabla p \rangle_i &= \sum_j (p_j - p_i) \nabla_i W_{ij} V_j = \Gamma_i (\nabla p)_i + 2 p_i \nabla \Gamma_i + \mathcal{O}(h). \end{cases} \quad (4.4)$$

In the previous expression, Γ_i and $\nabla \Gamma_i$ are responsible for a deviation from the exact differential operators. Therefore, in order to attain a correct field distribution, having Γ as close to 1 and $\nabla \Gamma$ as close to zero as possible becomes crucial. This is normally achieved with a regular particle distribution. Whilst a value different from 1 for Γ will result in an increase or decrease of the field intensity, $\nabla \Gamma$ is responsible of an unbalance in both magnitude and direction of the SPH operator. Hence, the correct computation of the term $2 p_i \nabla \Gamma_i$ represents a challenge for the algorithm to work.

The aim has to be to reduce the magnitude of $\nabla \Gamma_i$ as much as possible to recover the consistency of the SPH pressure operator and get a good initialization of the SPH scheme. The Particle Packing Algorithm is built based on that idea, i.e. initialize the particle distribution in a way such that $\|\nabla \Gamma_i\|$ is minimized. Vector $\mathbf{w} = -\nabla \Gamma_i$ points always in the direction of the maximum anisotropy in the particle distribution. Indeed, if the fluid domain is bounded and particles are not allowed to escape from the boundaries, $\mathbf{w}$ tends to fill all the asymmetries in the particle distribution, reducing its value as particle distribution is more regular.

Therefore, the first step to build the Particle Packing Algorithm is to close the domain boundaries, including those that will be later considered as free-surface in the SPH simulation. Fluid particles can be placed randomly, as they will be resettled during the particle packing algorithm. Nonetheless, how close are fluid particles to the equilibrium configuration might speed up the convergence of the algorithm. In Colagrossi et al. [2012], three options are studied: Cartesian, Triangular and Hexagonal grids. In this work, following Colagrossi et al. [2012], a Cartesian grid is used as initial particle distribution.

Once the domain boundaries are closed, and fluid particles set inside the fluid domain, the next step consists on assuming volumes (V_0), densities (ρ_0) and pressures (p_0) to be uniform over all

the fluid domain. For hydrostatic problems such as the ones that will be covered here, pressure is set as the maximum hydrostatic pressure $p_0 = \rho_0 g H$, H being the vertical span of $\Omega(t = 0)$. The pressure field being uniform implies that the continuity equation from Eqs. (2.1) can be removed, since it has no influence on pressure, and thus neither on the time evolution of the velocity field. Conversely, momentum equation becomes:

$$\frac{d\mathbf{u}_i}{dt} = -\beta \nabla \Gamma_i + \mathbf{T}_i. \quad (4.5)$$

Here, the factor β is a constant acting on the momentum equation, defined as $\beta = 2 p_0 / \rho_0$. This term acts like the source of the particle spatial reorganization. Normally, the larger p_0 is, the faster the particle resettlement acts [Marrone et al., 2013]. The term $\mathbf{T}_i$ is a damping force that is just used to ensure stability and thus convergence of the algorithm. A damping term of the form $\mathbf{T}_i = -\xi u_i$ is chosen here, with ξ defined as:

$$\xi = \alpha \frac{\sqrt{\beta}}{V_0^{1/d}}, \quad (4.6)$$

where d is the spatial dimension and α a free dimensionless parameter, set here as $5 \cdot 10^{-3}$, just in the same fashion as other damping terms for the initial settling used in the SPH literature (e.g. Monaghan [1994]).

The initial conditions for the Particle Packing Algorithm are obtained by setting particle velocities to zero and $V_0 = V_{\text{total}}/N$, where V_{total} is the total fluid volume and N the number of fluid particles. Finally, the time step is set as:

$$\Delta t = \text{CFL} \frac{V_0^{1/d}}{\sqrt{\beta}} \quad (4.7)$$

where the CFL value is set in this case always equal to 1.

The system described in Eq. (4.5) tends to converge towards a steady state in which $\mathbf{u}_i = 0$ and $\nabla \Gamma_i = 0$. When the steady state is assumed to be reached, the packing algorithm is stopped and the particle position's are used as the starting distribution for the standard SPH scheme. As a regular distribution is expected, the particle volume used for initialization can be assumed

to be constant, i.e. $V_i = V_0$. The initial particle pressure p_i is assigned by using a corresponding analytical expression (such as the hydrostatic solution in this case), and from there, density ρ_i is computed. Particle mass is obtained through $m_i = \rho_i V_i$.

4.2.1 Application case: a trapezoidal tank.

In order to test the algorithm implementation, an example is shown. Here, a trapezoidal tank is chosen, in the same fashion as in Colagrossi et al. [2012]. The aim is to investigate the capabilities of the SPH initialization algorithm to simulate the hydrostatic solution for different parameters and the two boundary formulations presented. The geometry can be seen in Figure 4.3, with all corresponding dimensions. In Figure 4.4 the initial Cartesian grid configuration

Figure 4.3: Schematic view of the trapezoidal tank geometry.

versus the initialization with the particle packing algorithm can be seen. Note how the free surface boundary is explicitly closed at this stage in order to obtain a regular distribution of particles.

In Colagrossi et al. [2012], several h/dr ratios are tested in order to assess the stability of the algorithm. From the conclusions extracted there, in present work a ratio of $h/dr = 2$ will be

Figure 4.4: Unevenness ($\nabla\Gamma$) for a Cartesian grid initial configuration (left) and after particle packing algorithm (right) for the boundary integrals methodology.

always used.

Figure 4.5 shows specific kinetic energy ($\mathcal{T} = \sum_i \|\mathbf{u}_i\|^2/2$) for both approaches at a fixed resolution of $H/dx = 50$. What is shown in this figure is the similarity between both approaches, with the remaining energy being the same for both of them. Also, the number of iterations needed to get this residual level is approximately the same both for ghost particles and boundary integrals. Therefore, it can be concluded that the algorithm performs analogously for both schemes.

In Figure 4.6, different resolutions for the boundary integrals approach are plotted. For all the tests performed, particle distribution tends to a stable value of specific kinetic energy. It is however noticeable that this value increases with resolution, indicating that it is more difficult for particles to attain a stable regime as their number increases. A similar effect has been found by Colagrossi et al. [2012]. However, in this work, once the stable value is reached, no further change is appreciated, regardless the number of iterations performed.

Moving on to the actual hydrostatic simulation, in which Navier-Stokes equations are solved (adding up the δ term to the continuity equation for stabilization purposes), Figure 4.7 shows the benefits of using the Particle Packing algorithm versus a solution with a Cartesian grid used as initial particle state. Whilst in the tank initiated with the Particle Packing algorithm the velocity field remains almost constant and zero, when the standard cartesian grid initialization

Figure 4.5: Specific kinetic energy evolution for $H/dx = 50$ for the trapezoidal tank. Blue dashed line represents ghost particle approach, whilst black solid line the boundary integrals approach.

Figure 4.6: Specific kinetic energy evolution for three different resolutions with the boundary integrals approach.

is used instead, greater velocity gradients are generated and free surface experiences spurious motions and irregularity after several iterations, turning the simulation even unstable at a certain point.

This observation is demonstrated by recording the maximum velocity at each time, showing hence kinetic evolution of both solutions, as it can be seen in Figure 4.8. Maximum velocity

Figure 4.7: Hydrostatic solution for the trapezoidal tank. Standard solution on the left and packing solution on the right. Normalized value of velocities are shown for two different initial configurations at $t\sqrt{g/H} = 10$. Resolution is chosen as $H/dx = 50$.

reached for the particle packing initialization is around 2 orders of magnitude below the standard initialization, and after a decreasing period (up to 40 non-dimensional time units), remains stable. On the other hand, the Cartesian initialization is not capable of keeping a homogeneous velocity profile and keeps oscillating and growing as time evolves.

Figure 4.8: Maximum velocity evolution for a Cartesian initialization (dashed blue line) and a Particle Packing initialization (solid black line).

The principal consequence of keeping a homogeneous velocity field is that the hydrostatic pressure profile and static configuration can be maintained. This is also a consequence of

keeping $\nabla\Gamma \simeq 0$. In Figure 4.9 the pressure field for the particle packing case can be seen, showing that it remains unperturbed for t equal ten times the typical time.

Figure 4.9: Hydrostatic pressure profile for the trapezoidal tank at $t\sqrt{g/H} = 10$. Resolution is chosen as $H/dx = 50$.

4.3 Free surface detection algorithm.

In order to track particles belonging to the free surface, a free surface detection algorithm is implemented. Additionally, tracking may serve as a basic step for further improvements regarding particle shifting in free-surface flows [Lind et al., 2012, Sun et al., 2017], where free surface has to limit motion in its normal direction, or further developments of physics at the interface, such as surface tension, e.g. [Huber et al., 2015], or phase change algorithms, e.g. [Das and Das, 2015]

There exist several alternatives in the literature, that can be based on the gradient of the kernel, on the number of neighbors or on the mass of the particles, if the mass is computed with the summation formula in Eq. (2.15) (for the different alternatives, examples can be found in [Marrone et al., 2010, Lind et al., 2012, Sun et al., 2017, 2019a]).

In present work, a free surface detection algorithm is implemented, based on the number of neighbors, inspired on the work by Marrone et al. [2010], and modified later by Sun et al. [2017,

2019a]. The choice of this approach to track free surface relies on the fact that in the presence of wall boundaries, values of the kernel gradient are different from the ones computed inside the fluid near the free surface, and this makes it complex to determine the threshold and even to compute the normal at the boundary. A procedure based on the particle's mass, as it is described by Green [2016], would be easier and cheaper from the computational point of view. Unfortunately, this choice would not allow to compute additional fields that might be needed for other implementations, such as the normal computation of free surface particles. Therefore, a more detailed approach is necessary.

The algorithm is based on two steps: in the first step particles near the free surface are detected applying the properties of the renormalization matrix introduced by Randles and Libersky [1996]:

$$\mathbf{B}(\mathbf{x}_i) = \left[\sum_j \nabla W_j(\mathbf{x}_i) \otimes (\mathbf{x}_j - \mathbf{x}_i) dV_j \right]^{-1}. \quad (4.8)$$

This way, the number of particles to be operated with in the following step decreases considerably. This method was first proposed by Doring [2005]. In this work, it was shown how the value of the minimum eigenvalue, λ , of the matrix $\mathbf{B}^{-1}$ depends on the spatial organization of the particles in the neighborhood of the i -th point. This eigenvalue tends theoretically to one inside the fluid domain, and to zero as the particle approaches a boundary. If the matrix $\mathbf{B}$ is computed over the fluid particles, boundaries are not included in the summation and eigenvalues of particles within the fluid near a boundary behave similarly as the ones near the free surface. To avoid it, the computation of $\mathbf{B}$ can be extended naturally to boundary terms, either with contour closure or fluid extension techniques.

Based on this definition, three regions in the fluid region $\mathbb{N}$ can be defined, establishing a threshold value for λ :

$$\left\{ \begin{array}{ll} i \in \mathbb{E} & \iff \lambda \leq 0.20 \\ i \in \mathbb{B} & \iff 0.20 < \lambda \leq 0.75 \\ i \in \mathbb{I} & \iff 0.75 < \lambda \end{array} \right. \quad (4.9)$$

The threshold value depends on the choice of the kernel function and the h/dx ratio. Here, the thresholds have been set for a ratio $h/dx = 2$ and the 5th order 2nd degree Wendland kernel

presented in Eq. (2.8). Therefore, particles belonging to $\mathbb{I}$, for which $\lambda > 0.75$ will be considered particles within the fluid domain, whilst particles within $\mathbb{E}$ will be automatically considered free-surface particles. For the particles belonging to the intermediate area $\mathbb{B}$, a second step is needed.

In the second step, it is necessary to define the normal of the fluid particles, in order to identify the truly free-surface ones. In Marrone et al. [2010], the algorithm is based on the fact that, inside the fluid domain, the sum of the kernel gradient over neighbors is very close to zero. When a particle instead is near the free surface, this sum is a good approximation of the local normal $\mathbf{n}$ to the free surface [Randles and Libersky, 1996]. Therefore:

$$\mathbf{n}(\mathbf{x}_i) = \frac{\mathbf{v}(\mathbf{x}_i)}{|\mathbf{v}(\mathbf{x}_i)|}; \quad \mathbf{v}(\mathbf{x}_i) = -\mathbf{B}(\mathbf{x}_i) \sum_j \nabla_i W_{ij} V_j \quad (4.10)$$

Conversely, in this work the approach developed by Sun et al. [2017] is followed, in which the normal is computed according to the following expression:

$$\mathbf{n}(\mathbf{x}_i) = \frac{\langle \nabla \lambda_i \rangle}{|\langle \nabla \lambda_i \rangle|}, \quad \langle \nabla \lambda_i \rangle := \sum_j (\lambda_j - \lambda_i) \otimes \mathbf{B}(\mathbf{x}_i) \nabla_i W_{ij} V_j \quad (4.11)$$

Once the normal is known, one can define a scan region (see sketch in Figure 4.10) defined by a set of constraints to find particles belonging to free surface region ($\mathbb{F}$). In 2-D, these conditions are:

$$\left\{ \begin{array}{ll} \forall j \in \mathbb{N} [|\mathbf{x}_{ji}| \geq \sqrt{2}h, \quad |\mathbf{x}_{jT}| < h] & \Rightarrow i \notin \mathbb{F} \\ \forall j \in \mathbb{N} [|\mathbf{x}_{ji}| < \sqrt{2}h, \quad |\mathbf{n} \cdot \mathbf{x}_{jT}| + |\boldsymbol{\tau} \cdot \mathbf{x}_{jT}| < h] & \Rightarrow i \notin \mathbb{F} \\ \text{otherwise} & \Rightarrow i \in \mathbb{F} \end{array} \right. \quad (4.12)$$

where $\boldsymbol{\tau}$ is the unit vector tangential to the free surface. Constraints become in 3-D:

$$\left\{ \begin{array}{ll} \forall j \in \mathbb{N} \quad [|\mathbf{x}_{ji}| \geq \sqrt{2}h, |\mathbf{x}_{jT}| < h] & \Rightarrow i \notin \mathbb{F} \\ \forall j \in \mathbb{N} \quad \left[|\mathbf{x}_{ji}| < \sqrt{2}h, \arccos \left(\frac{\mathbf{n} \cdot \mathbf{x}_{ji}}{|\mathbf{x}_{ji}|} \right) < \frac{\pi}{4} \right] & \Rightarrow i \notin \mathbb{F} \\ \text{otherwise} & \Rightarrow i \in \mathbb{F} \end{array} \right. \quad (4.13)$$

If any neighbor is located within the scan region, it means that there are fluid particles or solid boundaries in the normal direction. An additional area, that will be called free-surface region

Figure 4.10: Sketch of the scan region in 2-D. R1 corresponds to the search area of the first step, whilst R2 to the search area of the second step.

($\mathbb{A}$), is defined, composed by the particles within a $2h$ distance from the free-surface particles.

Figures 4.11 and 4.12 present successful examples of the algorithm applied to 2-D and 3-D geometries respectively. In Figure 4.11, top figure corresponds to the evolution of an elliptical (initially circular) patch of fluid (see Colagrossi [2005] for additional details of the case setup) and bottom figure corresponds to a 2-D dam-break case after impacting the wall. In both figures free surface is represented with black dots. Figure 4.12 represents a 3-D rectangular tank rotating around its roll axis. Free surface is colored in blue.

4.4 δ -LES-SPH model

As SPH method evolves towards a better understanding and solution of the Navier-Stokes equations, new methodologies arise, often inspired in schemes that are used in other frameworks and are adapted to the SPH methodology in order to overcome its shortcomings.

One of these examples can be found in Di Mascio et al. [2017], where the δ -SPH model is revisited from a LES perspective. The motivation comes from the fact that the simulation of problems at high Reynolds numbers still represents a challenge within the SPH context.

Figure 4.11: Free surface particles within region $\mathbb{F}$ for an elliptical patch of fluid (top) and a dam-break problem (bottom). Free surface particles are colored in black.

Figure 4.12: Free surface particles, colored in blue, for a 3-D rectangular rotating tank.

In standard SPH, DNS is usually performed. Hence, the resolution of all the scales involved in the problem becomes unfeasible if the Reynolds number is moderate or high. Similarly to what has been done in standard Eulerian methods, some attempts have been done towards RANS solutions (see e.g. Violeau and Issa [2007]) with moderate success. An alternative that is gaining attention in the last decade, known as Large Eddy Simulation (LES), becomes a feasible option in SPH for two reasons, mainly the extreme development of computer power and the fact that the filtering applied reminds somehow to the SPH convolutions. Therefore, Di Mascio et al. [2017] reinterpreted the LES formulation to fit the SPH nature, decomposing the LES filter into a spatial and a time filter. The resulting system of equations resembles the original SPH formulation, but taking into account the LES filtering into the dissipation terms, that now actually represent a real dissipation. This development has been later extended and applied to several cases by Meringolo et al. [2018, 2019], who carried out an energy balance to demonstrate the capabilities of the approach. The resulting system yields:

$$\begin{aligned}
\frac{D\rho_i}{Dt} &= -\rho_i \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla W_{ij} V_j + hc_s \sum_j \delta_{ij} \mathcal{D}_{ij} \cdot \nabla W_{ij} V_j \\
\frac{D\mathbf{u}_i}{Dt} &= \mathbf{g} - \frac{1}{\rho_i} \sum_j (p_i + p_j) \nabla W_{ij} V_j + hc_s \frac{\rho_0}{\rho_i} \sum_j \alpha_{ij} \Pi_{ij} \nabla W_{ij} V_j \\
\frac{D\mathbf{r}_i}{Dt} &= \mathbf{u}_i \quad p_i = c_s^2(\rho_i - \rho_0).
\end{aligned} \tag{4.14}$$

This system of equations is actually really similar to the standard δ -SPH scheme. However, the two diffusive terms in continuity and momentum equation can be regarded from a new physical perspective. First, the modified δ_{ij} quantity is written:

$$\delta_{ij} = 2 \frac{\delta_i \delta_j}{\delta_i + \delta_j}; \quad \delta_i = \frac{\nu_i^\delta}{c_s h}; \quad \nu_i^\delta = (C_\delta L_{LES})^2 \|\mathbb{D}\|_i \tag{4.15}$$

in which C_δ is a constant equal to 6.0 and L_{LES} is a reference length for the SPH filtering procedure, which is here set as the SPH spatial resolution, $L_{LES} = dr$, in the same fashion as the filtering window chosen in Eulerian methods. This choice implies that C_δ is different (although equivalent) to the one chosen in Di Mascio et al. [2017], where L_{LES} was set equal to the radius of the kernel, i.e. $L_{LES} = s \cdot h$

The quantity $\|\mathbb{D}\|_i$ is the Frobenius norm of the strain rate tensor $\mathbb{D}_i$ given by:

$$\|\mathbb{D}\|_i = \sqrt{2\mathbb{D}_i : \mathbb{D}_i} \quad (4.16)$$

where $\mathbb{D}_i$ is computed as:

$$\mathbb{D}_i = \frac{1}{2} \sum_j [(\mathbf{u}_j - \mathbf{u}_i) \otimes (\mathbb{L}_i \cdot \nabla W_{ij}) + (\mathbb{L}_i \cdot \nabla W_{ij}) \otimes (\mathbf{u}_j - \mathbf{u}_i)] V_j \quad (4.17)$$

Analogously, the viscous coefficient α_{ij} becomes a function of the interacting particles and is computed as:

$$\alpha_{ij} = \alpha + 2 \frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j} \quad \alpha_i = \alpha + \frac{K \nu_i^\alpha}{c_s h \rho_0} \quad \nu_i^\alpha = (C_\alpha L_{LES})^2 \|\mathbb{D}\|_i \quad (4.18)$$

in which C_α is the Smagorinsky constant, which takes the value of 0.12, and α is the contribution due to physical viscosity:

$$\alpha = \frac{K \mu}{c_s h \rho_0} \quad (4.19)$$

4.4.1 Application Case: dam-break case.

The dam-break problem has become a popular benchmark to test new aspects of liquid impact phenomenology [Abdolmaleki et al., 2004], also in the SPH context [Colagrossi and Landrini, 2003]. This problem was studied experimentally by Lobovsky et al. [2014], providing the community with a relevant amount of data, also used in this work. Initial setup of the problem is presented in Figure 4.13, where $d = 1$ for the range of tests presented in this work. With

Figure 4.13: Schematic view for the setup of the dam-break problem.

this test the intention is to show the performance of the δ -LES-SPH model in the context of free surface flows, including wave impacts and the investigation of energy dissipation. To this aim, different resolution results ($d/\Delta x = 100$, $d/\Delta x = 200$, $d/\Delta x = 400$) will be presented, computed with the current methodology, and compared to similar results carried out with the standard δ -SPH method and previous results obtained by Meringolo et al. [2019] for a fixed ghost particles methodology.

Figure 4.14 shows selected time instants of the flow after hitting the right wall.

Figure 4.14: Evolution of dam-break at different time instants. Color bar represents non-dimensional velocity. LES model with $d/n_y = 400$ particles and Mach number $Ma = 0.1$.

They are selected based on the values of the various terms in the energy balance, as presented in Figure 4.15. At initial time instants, up to 10 non-dimensional time units, kinetic and potential energy play the major role. At $t(g/d)^{1/2} = 3.0$ kinetic energy and potential energy reach a maximum and a minimum, respectively. Then, at $t(g/d)^{1/2} = 5.5$ a local extreme is reached,

corresponding to a time instant previous to the closure of the wave formed after the impact. Similarly, time instants $t(g/d)^{1/2} = 6.8$, $t(g/d)^{1/2} = 7.8$, $t(g/d)^{1/2} = 8.5$ and $t(g/d)^{1/2} = 9.3$ are selected because they correspond to a peak or a valley in the curve. In the evolution of the

Figure 4.15: Evolution of the different terms in the energy balance equation. LES model with $H/n_y = 400$ particles. ε_k corresponds to the kinetic energy, ε_p to the potential energy, ε_c to the compressible energy, and Q represents the dissipation coming from viscous and continuity sources.

flow, as the fluid starts being mixed, dissipation starts to gain importance. By the time instant corresponding to $t(g/d)^{1/2} = 10.0$, the global dissipation rate (represented by Q , being this the total contribution coming both from viscous and continuity sources) is sufficiently relevant to be considered as the major actor in the simulation. Mixing within the fluid has grown and vortices start to appear. With the LES model, if resolution is high enough, actual dissipation from viscous sources (translated into vorticity) can be regarded. Figure 4.16 shows a time instant of the vorticity field at $t(g/d)^{1/2} = 20.0$.

Figure 4.17 shows δ_i term at $t(g/d)^{1/2} = 9.4$, a moment in which δ_i has already reached a maximum value of $\delta_i = 0.2$ (which is a practical maximum limit to avoid non-physical behavior at impact times, according to Meringolo et al. [2019]) at several locations of the flow. The

Figure 4.16: Vorticity field at $t(g/d)^{1/2} = 20.0$. LES model with $H/n_y = 400$ particles and Mach number $Ma = 0.1$.

higher the δ_i value, the higher the instantaneous dissipation rate. As δ_i and α_i are linked by a proportionality relation, the latter would result in an equivalent figure at the corresponding scale.

Figure 4.17: Values of δ_i field at $t(g/d)^{1/2} = 9.4$. LES model with $H/n_y = 400$ particles and Mach number $Ma = 0.1$.

In Figure 4.18, values for δ_i and α_i obtained at different resolutions are compared to reference simulations performed by Meringolo et al. [2018] for the same test case, with a similar model and

Figure 4.18: Time evolution of momentum dissipation term Q_α and continuity dissipation term Q_δ for different resolutions, compared to the reference solution by Meringolo et al. [2019]

fixed ghost particles technique. As it can be seen, resolution plays a minor role on the dissipation terms, being relatively constant regardless the number of particles involved. Additionally, results obtained for the dissipation terms are compared to the standard SPH method in Figure 4.19, in which dissipation constants have been set to $\delta = 0.1$ and $\alpha = 0.01$. LES model agreement with the standard SPH solution is reasonable, especially at first stages, inducing greater dissipation from $t(g/d)^{1/2} = 10.0$ onward.

Considering how similar the results obtained are, it can be concluded that there is only a small effect coming from the boundary technique chosen. It is also possible to conclude that using a LES approach is equivalent to the standard δ -SPH scheme that has been used in SPH for a long time.

Finally, results obtained with LES solution are compared to experimental results. Pressure evolution at four different locations within the left wall (see Figure 4.20) are illustrated in Figure 4.21, comparing with LES solution obtained in this work. A good agreement is reached for all the sensors, showing that the current LES formulation combined with the boundary integrals technique developed in Chapter 3 has a wide range of potential future applications.

Figure 4.19: Comparison between dissipation terms obtained with standard SPH (solid red line) and LES-SPH (solid blue line). Resolution is $H/dr = 200$.

Figure 4.20: Geometry of the tank used in the experiments by Lobovsky et al. [2014] and location of pressure sensors. H in the experiment is set as $H = 300 \text{ mm}$. In this work, sensor's height has been scaled accordingly.

Figure 4.21: Pressure evolution obtained with LES solution for $H/dr = 200$, compared to experimental results obtained by Lobovsky et al. [2014]. Solid orange line corresponds to experimental results, and blue solid line to numerical results obtained in this work.

4.5 Phase change

As discussed in **Chapter 1**, phase change might be a relevant actor in sloshing flows under certain conditions. In particular, when liquid and vapor phases are in thermodynamic equilibrium, little variations of thermal conditions due to external sources or motions can result in relatively large variations of pressures due to phase change. This is especially relevant in several engineering applications, such as maritime transport of LNG or propulsion of launching rockets at upper stages. It seems hence desirable to include a phase change model that allows for a better understanding of the influence of the process in the global result. The phase change analysis has barely been studied in this context. Only some research carried out in the last few years by Arndt [2011], Behruzi et al. [2014] or Ancellin et al. [2016, 2018] can be found. Most of the works carried out up to this date are numerical simulations, due to the

hardly reproducible conditions for experiments, in which a little change in the local variables may produce considerable changes in the overall behavior of the system [Rose and Behruzi, 2014]. From the Eulerian perspective, several formulations have been proposed, such as those by Braeunig et al. [2010] Behruzi et al. [2014] and Ancellin et al. [2016]. The main drawback of the Eulerian approach when dealing with multiphase flow is the lack of resolution at the free surface when fragmentation due to breaking waves occur. Indeed, accurately defining the free surface is crucial in this problem as it is where the phase change takes place.

On the other hand, a few attempts have been made following Lagrangian formulations, such as SPH. A few studies involving phase change in different conditions and at different stages, such as solidification and melting [Monaghan et al., 2005], or evaporation and condensation [Das and Das, 2015] have been carried out.

In order to deal numerically with phase change rates, models based on pressure variations at the interface are a popular option. In particular, the Hertz-Knudsen model, introduced by Hertz [1882] and Knudsen [1915], appears as the simplest and most effective approach to carry out this analysis. The Hertz-Knudsen model reads:

$$\dot{m} = A_{int} \sqrt{\frac{M}{2\pi R_u}} \left(\alpha_e \frac{p_{sat}}{\sqrt{T_{sat}}} - \alpha_c \frac{p_{gas}}{\sqrt{T_{gas}}} \right), \quad (4.20)$$

where $\dot{m}$ is the rate of mass per unit time, A_{int} is the interface area, M is the molar weight of the gas phase, R_u is the universal gas constant, α is the accommodation coefficient, with a subscript c indicating condensation and a subscript e indicating evaporation, p_{gas} is the gas pressure and p_{sat} the saturation pressure, T_{gas} is the gas temperature and T_{sat} the saturation temperature.

This expression arises from a description based on the Kinetic Theory on Gases (for more information, see Carey [1992]), that allows to determine the highest flux possible in a phase change process. The accommodation coefficients act in the Hertz-Knudsen model as limiters of the phase change and their only constraint is to be less than or equal to one. They can be regarded as the representation of the fraction of molecules which change of phase upon striking the liquid-vapour interface. These coefficients are not known *a priori* and have to be found

based on experimental results or numerical validation. Indeed, they are necessarily introduced to fit the theory with the experimental results.

In order to reproduce the physics involved in phase change, the energy equation has to be added to the governing equations presented in Eq. (2.1). If we assume that $de = \rho c_p dT$, one can write the energy equation as a function of temperature in the following form:

$$\rho c_p \frac{dT}{dt} = \nabla \cdot (\kappa \nabla T) - p \nabla \cdot \mathbf{u} + \phi_v + Q, \quad (4.21)$$

where the first term on the RHS is due to conduction and the second term is the compressibility effect which is taken into account due to the weakly-compressible nature of the SPH method. c_p is defined as the specific heat at constant pressure and κ the thermal conductivity. Viscous heating (ϕ_v) is assumed to be negligible compared to heat conduction and therefore no viscous term will be modeled here. Q is a source term included in order to account for radiation and other effects not considered in the previous terms. However, this work will not consider any source apart from conduction and compressible effects and hence this term will not be modeled either.

4.5.1 Numerical model for evaporation and condensation within a single phase SPH scheme: algorithm description

The idea is to introduce a new formulation, in which the dynamics and thermodynamics of the liquid are solved, while the gas phase role in the flow is assumed to be modeled with sufficient accuracy assuming homogeneous values for the thermodynamic variables.

This main assumption in the model is justified based on: first, the fact that the speed of sound in the gas is large enough to allow pressure changes induced in the interface to be transmitted to the gas phase in time scales much shorter than the ones in the sloshing phenomena. Second, on assuming that the thermal gradients are relevant only in the thermal boundary layer at the interface while an average temperature can be assumed to represent this scalar in the bulk of the gas phase region. This second assumption is based on the fact that convective effects on the gas are large enough to spread the temperature over the gas volume at the same time.

Based on these assumptions, the current approach will be shown to be reasonable and to render accurate results while considerably reducing the computational effort. Similar approaches have been reported in the literature for engineering applications (as in e.g. Migliore et al. [2017]). The model is valid to reproduce evaporation and condensation phenomena in tanks with the conditions explained above. The sequence of events that take place are:

Figure 4.22: Sketch and geometric details of the implemented phase change model.

1. The initial condition consists of a liquid phase filled up to a certain level (X_0). The rest of the volume of the tank is assumed to be vapor phase. Both phases are at saturation conditions and in thermodynamic equilibrium between them and with the tank walls. The interface is assumed to keep this condition any time during the simulation.
2. There is a heat flux q_w being applied to the system through the walls. This heat flux affects more rapidly the gas than the liquid, as thermal inertia in the gas phase is smaller than in the liquid phase. Hence initially the liquid can be assumed not affected by this heat flux q_w .

3. The heat flux applied through the walls produces an increase in the gas temperature, which is the phase with smaller thermal inertia. Gas properties are assumed uniform throughout the space. Hence, the gas temperature varies each time step according to:

$$\frac{dT_{\text{gas}}}{dt} = \frac{q_w A_q}{C_v m_{\text{gas}}} , \quad (4.22)$$

where A_q is the area of the tank wall where heat transfer occurs, C_v the specific heat coefficient at constant volume and m_{gas} the mass of the gas phase.

4. This variation in the gas temperature is translated into a variation of the gas pressure according to the equation of state for an ideal gas:

$$p_{\text{gas}} = \rho_{\text{gas}} R_{\text{gas}} T_{\text{gas}} , \quad (4.23)$$

where p_{gas} is the pressure of the gas and R_{gas} the gas constant, which depends on the molar mass of the species considered.

5. The rise in gas temperature causes the saturation temperature of the interface to change since the interface tends to be in equilibrium with the temperature distribution in the ullage gas. Therefore, the saturation temperature changes as:

$$\frac{dT_{\text{sat}}}{dt} = \frac{q_{\text{iv}} A_{\text{int}}}{C_l m_{\text{int}}} , \quad (4.24)$$

where A_{int} is the area of the interface between the liquid and the gas phase, q_{iv} the heat flux through the interface and m_{int} the mass of the liquid at the interface. This kind of averaged models have practical interest since they are used for, *e.g.*, studying the weathering of LNG, *i.e.*, how the composition of LNG changes in time when stored [Migliore et al., 2017].

The heat flux at the interface can be defined as:

$$q_{\text{iv}} = - \kappa_l \frac{\Delta T}{\delta_T} = -k_l \frac{T_{\text{gas}} - T_{\text{sat}}}{\delta_T} , \quad (4.25)$$

where κ_l is the liquid phase thermal conductivity and δ_T the thickness of the thermal boundary layer.

6. The increase in the saturation temperature leads to an increase of the saturation pressure, which is modeled through the Clausius-Clapeyron relation as:

$$p_{\text{sat}} = \exp \left[- \left(\frac{\Delta H_v}{R_{\text{gas}}} \right) \frac{1}{T_{\text{sat}}} + B \right], \quad (4.26)$$

where ΔH_v is the specific latent heat of vaporization of the liquid, R_{gas} is the gas constant and B is a constant obtained from a point of the coexistence curve in the pressure-temperature phase diagram [McQuarrie and Simon, 1997].

7. Once all the fields are known, the Hertz-Knudsen model can be applied as from Eq. (4.20). Depending on the sign of this rate, there will be condensation or evaporation. According to the expression, a positive rate implies evaporation, as the gas mass increases, and a negative rate implies condensation. Accordingly, the mass of the liquid at the interface will change.
8. Finally, the new mass in the gas phase can be computed for the following time step.

4.5.2 SPH Implementation

The different terms that are considered within the temperature equation (Eq. (4.21)) are discretized in the SPH formalism as:

$$c_p \left. \frac{dT}{dt} \right|_i = \frac{1}{\rho_i} \left(\sum_j \Theta_{ij} \nabla_i W_{ij} V_j + \sum_j p_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} V_j \right), \quad (4.27)$$

where, similarly to Π_{ij} , Θ_{ij} is defined as:

$$\Theta_{ij} := (k_i + k_j) \frac{(T_j - T_i) \cdot \mathbf{r}_{ji}}{\|\mathbf{r}_{ji}\|^2}, \quad (4.28)$$

If mass transfers at the interface are large enough, liquid particles may have to be removed or added in order to accomplish liquid mass and volume requirements set by the evaporation-

condensation algorithm. These transfers occur only at the interface of the liquid, and they are hence to be accounted for by the particles that have been detected with the free surface detection algorithm presented in Section 4.3.

However, imposing mass changes directly on fluid particles will inevitably imply a change in the compact support volume and hence a multi-resolution approach will be needed. This would be a possible approach that can be developed at a later stage. Nonetheless here, in order to overcome this complexity, mass exchange will be stored within some “interface” particles, in the same fashion it is done by Das and Das [2015]. When the mass-exchange value reaches the particle mass, a particle is added or removed (depending on the sign), with an equal probability distribution across the free-surface.

4.5.3 Stefan Problem Benchmark

In order to validate the model presented in this work, two different simulations of a benchmark test will be performed in first place. The benchmark is based on the well known one-dimensional Stefan problem reformulated for the interaction between a liquid and a gas [Hu and Argyropoulos, 1996], and adapted in order to reproduce the physics as set in the model. This is basically a moving boundary problem which is here modeled according to the following set of equations:

$$\frac{\partial T_{\text{gas}}}{\partial t} = \frac{q_w A_{\text{int}}}{c_{v,\text{gas}} m_{\text{gas}}}, \quad (4.29)$$

$$\kappa_l \frac{T_{\text{gas}} - T_0}{\Delta x} = H_v \rho_l \frac{dX}{dt}, \quad (4.30)$$

$$m_{\text{gas}} = A [\rho_l X + (\rho_{\text{gas}} - \rho_l) X_0], \quad (4.31)$$

where the subscripts “l” and “gas” refer to the liquid and gas phases respectively, T_{gas} is the gas temperature, κ_l is the thermal conductivity of the liquid phase, H_v the latent heat of vaporization, T_0 the saturation temperature, and X the position of the interface.

Eq. (4.29) models the temperature of the gas phase changing with time due to a wall heat

Table 4.2: Methane bulk physical parameters

Phase	c (J/ (K kg))	ρ (kg/m ³)	κ (W/ (K m))	D (m ² /s)	H_v (J/kg)
Liquid	3299	420	0.21	1.55×10^{-7}	$5.1 \cdot 10^5$
Vapour	2260	1.75	0.025	1.8×10^{-5}	$5.1 \cdot 10^5$

flux q_w , but assumed, as already discussed, uniform within the gas region. This temperature reference displaces the interface location X depending on the sign of the heat flux onto the interface, according to Eq. (4.30). This flux is estimated as proportional to the temperature change from the gas to the interface over an inter-facial region of width the kernel smoothing length, h . Finally, mass is transferred between phases according to Eq. (4.31). This formulation differs from the usual Stefan problem by assuming constant temperature in the gas phase, and a process at constant volume (instead of the more common constant pressure.)

In order to compare the solution to the one provided by the method presented in this work, Eqs. (4.29), (4.30) and (4.31) are solved numerically. The physical constants are the ones corresponding to liquid methane and its vapor phase, which are summarized in Table 4.2.

AQUAgpusph was not designed to perform one-dimensional simulations. Hence, a two-dimensional domain is adapted to this one-dimensional problem. The geometry is the same as the one shown in Figure 4.22. A symmetry condition is assumed at the side boundaries, the bottom boundary is set at a temperature T_0 and a heat flux q_w is applied in the upper boundary. Depending on the direction of this heat flux, the temperature of the gas phase will increase or decrease, therefore inducing evaporation or condensation. The position of the interface is called X , being X_0 , the initial height position at time $t = 0$.

An evaporation case is simulated first. According to the Hertz-Knudsen equation (Eq. (4.20)), simulations are performed for different values of the accommodation coefficients α_i and compared with the theoretical solution with $q_w = 6 \text{ W/m}^2$. Same values of the accommodation coefficients (α_e and α_c) are used to account for the influence of evaporation and condensation according to Eq. (4.20). The initial value for the pressure is atmospheric pressure, $P = 101 \text{ kPa}$, which is the saturated pressure at the boiling temperature $T_0 = 111 \text{ K}$. The initial value of X is $X_0 = 10^{-3} \text{ m}$. Figure 4.23 shows dimensionless time evolution versus dimensionless

Figure 4.23: Results for the variation of the interface for the evaporation benchmark. The red line indicates the theoretical solution, whilst the green and black lines the results for an accommodation coefficient, α , of 10^{-4} and 5×10^{-4} respectively.

variation of the position at the interface. Time is scaled by the characteristic time (τ) that would be needed theoretically to evaporate a discretized part of the domain (Δx) as a function of the initial temperature T_0 , the enthalpy of vaporization H_v , the initial position of the interface (X_0), the density (ρ_l) and the thermal conductivity (κ_l) of the liquid, according to

$$\tau = \frac{H_v \rho_l X_0 \Delta x}{\kappa_l T_0}. \quad (4.32)$$

The position of the interface is represented as a function of the initial position of the interface. As it can be seen from Figure 4.23, the theoretical solution lies between two SPH solutions obtained with $\alpha = 10^{-4}$ and $\alpha = 5 \times 10^{-4}$, which suggest this is the range in which a reasonable value of the accommodation coefficient can be defined.

Results of mass transfer obtained by the method here proposed for SPH are presented as interface variations following Eq. (4.33):

$$X = \frac{\dot{m}}{A_i \rho_{\text{liq}}} t. \quad (4.33)$$

Analogously, the performance of the method for a condensation situation has been tested. The geometry employed is the same as before, however flux now points outwards and therefore $q_{mr} = -6 \text{ W/m}^2$. For this case the interface is slightly separated from the wall and $X_0 = 0.01$

Figure 4.24: Results for the variation of the interface for the condensation benchmark. The red line indicates the theoretical solution, whilst the green and black lines the results for a value of the accommodation coefficient, α , of 5×10^{-5} and 10^{-4} respectively.

m. Initial temperature and pressure values are the same as in the previous case. Results are depicted in Figure 4.24, showing a reasonable agreement for a value of the accommodation coefficient of 5×10^{-5} . Values are represented in non dimensional form as it was done for the evaporation test.

From the results obtained, several remarks can be done. First of all, it can be appreciated that there is a strong influence of the accommodation coefficient α in the results. However, this dependency was expected, relying in previous works which used the same approach for the calculation of the mass rates, such as the ones of Behruzi et al. [2014] or Ancellin et al. [2016]. Another important aspect is the quantitative value of the α coefficient used. If compared with other numerical results, the range of values that fits the theoretical solution is slightly lower than the ones expected according to the results obtained from other analysis. However, there exists a lot of controversy around the range of values that the accommodation coefficient should lie on, and nowadays the values obtained depend mainly on the conditions of the problem tested [Persad and Ward, 2016].

The values of the accommodation coefficient here obtained lie in the same order of magnitude for both evaporation and condensation processes, and both fit reasonably well the analytical solution. Moreover, quantitative results are also in the same range of values for both test cases. Low values of variation of the interface with respect to the initial position are found. This is

due to the slowness of these phenomena if temperature gradients are not excessively high, as it is the case here.

Two accommodation coefficients have to be fixed for each simulation. Same values of α_e and α_c are used in this work, so the expression for the mass transfer (4.20) might be further simplified to only consider one accommodation coefficient. However, it seems reasonable to keep both coefficients in the formulation as the influence of both processes may be different depending on the application, despite it being difficult to quantify such influences. Further analysis is therefore needed in this direction.

4.5.4 2D-Application Case

Several engineering applications may be sensitive to the addition of thermal effects to be coupled with the standard Navier-Stokes equations for solving fluid motion. The case of interest here is the influence of the thermal effects when sloshing motion occurs in fluids carried at cryogenic temperatures, which are carried in equilibrium with its vapour phase and might be pressurized.

Therefore, a 2D simulation of a sloshing tank, including these thermal effects is performed. A sketch of the geometry is shown in Figure 4.25. This geometry is a standard simplified version of the ones used for the simulation of sloshing in LNG carriers. The length of the tank is $L = 1$ m, the height $D = 0.5$ m, and the initial filling height of the liquid $H = 0.1$ m. Methane is chosen for this simulation, using the same values as for the benchmark test (see Table 4.2).

The center of rotation of the tank is set at 0.47 m and the motion is a sinusoidal motion of amplitude $A = 0.05$ m and angular velocity $\omega = 1.5$ rad/s.

As has been seen, evaporation and condensation are dependent of the temperature gradient in the tank. Therefore, in order to force evaporation, a heat flux of $q_w = 6$ kW/m² is applied at the top wall. Results for the gas mass variation in the tank as a function of time as well as pressure evolution of the gas phase are presented in Figure 4.26. Mass evolves similarly to the interface evolution presented in Section 4.5.3 for the benchmark test case.

A detail of the evaporation algorithm is shown in Figure 4.27, where a comparison is shown between simulations with and without the evaporation model. The mass of the particles at the

Figure 4.25: Geometry for the sloshing tank tested

Figure 4.26: Evolution of the mass and pressure in the gas phase for the sloshing tank. Mass is normalized by the initial mass, pressure by the initial gas pressure, whilst time is scaled according to the characteristic time τ

free surface is reduced as the gas mass increases due to the heating of the tank. When this mass is reduced enough, particles are removed from the free surface.

Figure 4.27: Detail of the evaporation at the liquid free surface for the sloshing tank. Left figure corresponds to a simulation without the evaporation model implemented and right figure corresponds to a simulation where evaporation occurs.

Chapter 5

Applications

In this Chapter, the new implementations will be applied to a set of selected applications.

Three application cases are presented: first, a general 3-D benchmark, consisting on a dam-break benchmark case will be analyzed from different numerical perspectives in order to assess improvements of the new boundary integrals formulation.

Second, the formulation is extended to a moving frame of reference case, consisting of an anti-roll tank. With this case, the aim is to demonstrate applicability of the methodology to a general 3-D engineering case, comparing results on the global moment measurement in a complex geometry versus experimental results.

Finally, an application test within the aeronautics industry will be shown. Despite being a 2-D case, the complexity of the motions involved, and particular cornered geometry makes it a very challenging application that is thoroughly analyzed.

5.1 3-D dam break

In order to assess the performance of the new boundary integrals methodology (introduced in Section 3.4 and applied to a 2-D geometry in Section 3.4.4) in a more general context, the SPHERIC validation test number 2, consisting on a 3-D dam break flow, is here considered. This validation test has already been used by other authors, such as Mayrhofer et al. [2015] and Violeau et al. [2014].

The 3-D dam break initial condition is schematically depicted in Fig. 5.1. A reservoir of water

Figure 5.1: Schematic 3-D dam break flow initial condition Kleefsman et al. [2005]

with the shape of a rectangular box, with dimensions $1.228 \text{ m} \times 1 \text{ m} \times 0.55 \text{ m}$, is initially set in hydrostatic equilibrium at one side of the tank, which has dimensions $3.22 \text{ m} \times 1 \text{ m} \times 1 \text{ m}$. A fixed box of dimensions $0.161 \text{ m} \times 0.403 \text{ m} \times 0.161 \text{ m}$ is also placed inside the tank.

The experiments on this test case were documented by Kleefsman et al. [2005]. In such experiments the wave height was measured by the vertical probes labeled H_1 - H_4 . An additional set of pressure sensors were distributed along the fixed inner box, as schematically depicted in Fig. 5.2.

To carry out the simulations, a numerical sound speed of $c_s = 40 \text{ m/s}$ is considered, as well as the typical water density and viscosity values, $\rho_0 = 998 \text{ kg/m}^3$ and $\mu = 10^{-6} \text{ m}^2 / \text{s}$. The δ -SPH formulation of Antuono et al. [2012] is applied for stability, following Fatehi and Manzari [2011] (see also Cercos-Pita et al. [2016], where several δ -SPH term alternatives are discussed.) This is in contrast with the simulations carried out by Violeau et al. [2014] and Mayrhofer et al. [2015], where a large artificial viscosity was considered in order to preserve the stability. In those works, experimental records were not included, and SPH results were compared against a Volume-of-Fluid Finite Volume simulation.

No-slip boundary conditions have been imposed along the solid walls. However, in this practical application a boundary force is added as well, to avoid walls penetration. It is triggered when

Figure 5.2: Schematic inner box description [Kleefsman et al., 2005]

a fluid particle moves closer than $0.1 \Delta r$ to the wall. Even though such a boundary force has a detrimental effect in the pressure record noise, it is nevertheless required to avoid dramatically small time steps.

The air phase is neglected, for optimization purposes, assuming the inconsistencies close to the free surface discussed by Colagrossi et al. [2009] and Colagrossi et al. [2011] which have been also discussed previously in Section 3.4. Besides the consistency issues close to the free surface, neglecting the air phase may induce some other errors in the pressure records, as already mentioned by Mayrhofer et al. [2015].

In order to analyze the effect of the discretization on the results, several initial particle spacings have been considered, $\Delta r = 0.55/30$ m, $0.55/45$ m, and $0.55/60$ m, with a constant kernel length ratio, $h/\Delta r = 4$. Along the same line, several kernel lengths have been simulated, with a spacing of $\Delta r = 0.55/45$ m, namely $h/\Delta r = 2, 3$ and 4 .

In Fig. 5.3, the pressure records computed with this thesis implementation of AQUAplusph are compared with the experimental ones, for different initial particle spacing values.

Pressure records are obtained with a 1000 FPS sampling rate. High frequency noise in the SPH solution has been filtered out by means of a Savitsky-Golay filter [Savitzky and Golay, 1964].

After time $t = 0.5$ s, the pressure record associated to spacing $\Delta r = 0.55/45$ is significantly affected by a ~ 100 Hz frequency noise signal, whose origin is not clear.

Nevertheless, a good agreement in the pressure measured at the pressure probes P_1 and P_2 is achieved for all the simulations, considering that SPH tends to overestimate the pressure peak at sensor P_1 . The same cannot be said for the pressure sensors P_3 and P_4 , where the phenomenon is poorly captured in the simulation.

Figure 5.3: Pressure validation for different initial particle spacing values.

The overestimated pressure peaks, as well as the errors at P_3 , have been attributed in the past to the absence of the air phase, see e.g. Mayrhofer et al. [2015]. Unfortunately, the predictions for the P_4 pressure record, which is consistently the one most affected by the neglect of the air phase, have been circumvented in the SPH literature [Crespo et al., 2011, Lee et al., 2010, Mayrhofer et al., 2015, Violeau et al., 2014]. Anyway, given the accuracy of the records at probes P_1 and P_2 , and the large errors at P_3 and P_4 , it is plausible to conclude that the air phase plays an important role in the experimental pressure.

In Fig. 5.4 similar pressure validations are shown for different kernel length ratios and constant initial particle space, $\Delta r = 0.55/45$ m.

The number of neighbors plays so far a secondary role in the computed pressure at sensors P_1 - P_2 . However, the reduction of the kernel length, and therefore the smoothing radius, improves the pressure at P_4 , specially close to the pressure peak, even if it always poorly captured in SPH.

Again, the simulation associated to the parameters $\Delta r = 0.55/45$ m and $h/\Delta r = 4$ is significantly affected by a ~ 100 Hz noise signal, which is not seen for the other lengths at all.

Additionally, Figure 5.5 shows the corresponding height probes at locations H_2 - H_4 (for the times shown, probe at location H_1 is negligible). It can be appreciated that correspondence between numerical simulations and experimental results is in great accordance regardless the

Figure 5.4: Pressure validation for different kernel length ratios

resolution tested.

Figure 5.5: Height validation for different initial particle spacing values.

From the results discussed above, it is reasonable to suggest that simulations are correctly converging, both when the particle spacing is decreased and when the number of neighbors is increased.

As stated above, the computational performance can be a critical factor, as already already stressed in Ref. Violeau et al. [2014], where the computation of the analytical value of γ took 40% of the overall computation time. In Table 5.1, the time required to compute a single time

step, in a NVIDIA GeForce GTX 750 Ti graphics device, is presented for all the simulations described above, for the traditional and the new γ formulations. Additionally, the performance for $\gamma = 1$, i.e. when the factor is not computed at all, has been added in order to be able to evaluate the overall impact. The traditional γ formulation takes $\sim 10\%$ of the overall

Table 5.1: Time in seconds to compute a single time step, averaged along the first 100 time steps.

Δr (m)	$h/\Delta r$	Former formulation	New formulation	$\gamma = 1$
0.55/30	4	0.89	0.84	0.80
0.55/45	4	2.95	2.82	2.68
0.55/60	4	7.24	6.93	6.62
0.55/45	2	0.50	0.48	0.43
0.55/45	3	1.37	1.28	1.18

computational time when large number of neighbors is considered, growing up to $\sim 16\%$ for the lowest number of neighbors, $h/\Delta r = 2$. The new formulation requires almost half the time for the largest number of neighbors, i.e. $\sim 5\%$ of the overall computation time. Such number rises to $\sim 10\%$ for the lowest number of neighbors. The general reduction of the computational cost, when the new formulation is applied, reflects the benefit of moving from a volume integral to a surface one.

For completeness, it is interesting to compare the results obtained with the new formulation, with the ones obtained in Lee et al. [2010], where incompressible-SPH (ISPH) was applied. In Fig. 5.6 the pressure records at the sensors P_1 and P_3 , for the ISPH simulation and the WCSPH simulation with the new formulation are depicted, and compared with the experimental results. In this particular case, WC-SPH has been able to capture significantly better the flow impact phenomena.

5.2 Anti-roll tank (ART)

A very relevant application of sloshing is the design of Tuned Liquid Dampers (TLD). In a general context, they can be defined as systems that help in minimizing motions coming from an external input taking advantage of the motion of liquid inside them.

Figure 5.6: Pressure comparison with an ISPH solution

A particular application of TLDs can be seen in the naval industry with anti-roll tanks (ART), which are devices that help in reducing roll motion due to waves for ships at sea. The design principle of ARTs is based on the moment that the fluid moving inside the tank generates, that counteracts the rolling motion induced by waves to the ship. In order to cover different operational conditions, the tank filling level can be varied. Each filling level covers a range of frequencies at which the tank best operates.

In this section, a simulation of the full range of operational frequencies of a ship is carried out. The ship is a multi-purpose vessel of $L = 88.5\text{ m}$ and $B = 18.4\text{ m}$ and the tank to be installed has the dimensions presented in Table 5.2. Center of rotation is located 2.27 m over the base line. Filling level is chosen as 1.30 m , that corresponds to a 50% filling level condition. Baffles are set such that blockage factor corresponds to 0.5.

Table 5.2: Main dimensions of the anti-roll tank

Dimension	Value (m)
Length (L)	4.5
Breadth (L)	18.0
Moulded depth (D)	2.56
Baffles location from the center-line	4.73

Figure 5.7: Anti-roll tank laboratory at CEHINAV (UPM) where the experiments are carried out. Source: www.canal.etsin.upm.es

Pure roll experiments for this tank are carried out at scale 1 : 21.9 at CEHINAV facilities. The tank is placed on a device that rotates around an axis with fixed amplitude and a selected frequency. Figure 5.7 shows the device with a tank on it. A picture of the tank tested at CEHINAV facilities is shown in Figure 5.13.

Moment amplitude is measured with extensimetric gauges, whilst for the motion signal a potentiometer is used. Signals are filtered with a low-pass filter and maximum amplitude of both signals and phase lag between them are recorded at a frequency range from 0.39 rad/s to 0.90 rad/s (values are given at full scale, scaled appropriately from frequencies tested at the experiment). It is worth mentioning that these measures are taken for a single period, that has been chosen once the tank has performed several periods at the selected frequency. This is important, as it will be shown later, because both moment amplitude and phase lag values might slightly vary from one period to another.

SPH simulations for the same tank, at full scale, are also carried out. Speed of sound is set at $c_s = 25 \text{ m/s}$ and particle distance $dr = 0.1 \text{ m}$, giving in total a number of particles around 140000.

Figure 5.9 shows moment signal recorded from the SPH simulations for a frequency $\omega = 0.63$

Figure 5.8: Geometry of the tank tested.

rad/s. Results are presented here as raw data, without any filtering process. As it can be appreciated, at peak times high frequency spurious values for moment are recorded. It can also be observed that the output moment signal is not constant at every period. Even though a ramp has been applied for the first period in order to smooth the first stages, this changing behavior in peak values is shown even far from the initial periods. This can give an idea of the stochastic behavior of sloshing motion in this case. Moment signal is filtered in the same fashion as in the experiments, in order to obtain a comparable curve. Once the signal is filtered, phase lag from the simulations, is obtained through a cross correlation process. Figure 5.10 shows the filtering procedure carried out, where higher frequency components are removed from the signal, while keeping the main component at the desired oscillating frequency. Top image shows the original unfiltered signal, middle picture the fast Fourier transform (FFT) that is applied

Figure 5.9: Moment amplitude signal for a simulation with $\omega = 0.63$ rad/s.

to identify and remove high frequencies, and bottom figure shows the comparison between the original and the novel filtered signal. Results for the moment amplitude and the phase lag are presented in Figure 5.11, where the simulation results are compared to the experimental ones.

Results show in general a good agreement between experiments and numerical simulations. Regarding phase lag, the most accurate results are obtained at the operating range of the tank, between 0.6 and 0.7 rad/s, and they lose accuracy as they move away from this range on both lower and higher frequencies, maintaining reasonable values in any way.

Moment amplitude curves follow a similar trends. They keep at constant values for frequencies below 0.6 rad/s and amplitude starts to decrease from this frequency to higher frequencies. Bigger discrepancies are found in the moment amplitude regarding quantitative results, even though maximum error, found at 0.7 rad/s, is around 10%. In order to check curves properly, simulations at higher resolution would be needed. Additionally, a deep analysis in the experiment should be done, recording several periods to have a better measure of moment amplitude and phase lag variations between periods.

Figure 5.10: Filtering procedure followed for output moment signal from simulations. Top graph shows the original signal, middle figure its FFT before and after the filtering, and bottom picture shows the filtered signal compared to the original one.

5.3 Vertical sloshing

5.3.1 Description of the problem

Challenges in aerospace industry, especially linked to the increase in passenger aircraft's size, demand further research of associated systems that might influence craft behaviour when in operation. In particular, there is an interest in optimizing the wings of large civil passenger aircraft, which are designed to withstand the loads due to atmospheric gusts, turbulence and even landing impacts. In this section, the aim is that through the investigation of the damping effect of sloshing on the dynamics of such wings, in which the fuel is normally stored, and also through optimization of their inner configuration and the analysis of liquid filling level, this goal could be achieved.

Sloshing has been proved to be effective in dampening movements in analogous structures. These ideas have lately been considered within the aerospace industry for propellant rocket

Figure 5.11: Results for the simulations carried out, compared to the experimental results. Top graph represents the moment amplitude, and bottom graph the phase lag. Blue line represents experimental results and green line simulation results

tanks (see e.g. Arndt and Dreyer [2008]) or in preliminary studies on sloshing on aircraft fuel tanks [Gambioli, 2009].

In this work, the intention is to continue with those preliminary studies and to extend the knowledge on damping effects due to sloshing on aircraft wing tanks by analyzing the use of fuel slosh to reduce the design loads on aircraft structures.

SPH will be used as the numerical tool to reproduce sloshing. Previous analyses of this problem have been carried out by Bulian et al. [2010], Bouscasse et al. [2014a] and Bouscasse et al. [2014b], where a dynamical system consisting on an oscillating tank filled with fluid is studied. These works focus on understanding energy dissipation mechanisms, and a non-linear model for motion is used. Similarly, in this work the SPH tool will be complemented by a set of numerical models that reproduce wing motion that are coupled to the SPH computed sloshing loads.

The goal consists of reproducing liquid loads on wing tanks within the aircraft, and assessing their impact on motions and whether additional damping due to the liquid presence might be induced. With that in mind, an experimental campaign was carried out at the Airbus Proto-

Figure 5.12: Set-up of the experiments carried out at Airbus Protospace Lab in Filton (UK).

space Lab in Filton (UK) (see Titurus et al. [2019], Gambioli et al. [2019]). The preliminary arrangement can be seen in Figure 5.12. The test consists on the wing represented by a cantilever beam with a liquid tank attached at its tip. The beam is preloaded and released, and the accelerations at different points are recorded. Also the liquid motion is visually recorded at high speed rates in order to understand liquid slosh inside the tank. Different configurations were used, including different liquids, inner baffled configurations (both horizontally and vertically located) and various filling levels. In order to reproduce results of the experiment, two options are chosen to move the tank: the most straight-forward possibility is to force motion with output data obtained from the experiments. The other option is to develop a numerical model of a fully coupled fluid-structure interaction problem. The structure is modelled through the Euler-Bernoulli beam theory and solved by different means. Numerical methods such as finite elements or SPH are avoided, and instead the beam is modeled by a simple mass-spring-damper system and by modal analysis [James et al., 1994]. For the fluid, the δ -LES-SPH model developed in this work is used.

Due to the complexity, a set of preliminary tests is presented in order to understand every phenomenon associated.

5.3.2 Coupling: Beam model

The equation for a beam is given by the Euler-Bernoulli beam theory as:

$$m(x)\frac{\partial^2 w(x,t)}{\partial t^2} + c\frac{\partial w(x,t)}{\partial t} + EI\frac{\partial^4 w(x,t)}{\partial x^4} = f(x,t), \quad (5.1)$$

where x is the spatial coordinate, t the time, $m(x)$ is the distributed mass of the beam (in the future the mass will be assumed as a constant distribution $m(x) = m$), w the vertical displacement, c accounts for the internal damping of the beam, EI is the structural rigidity and $f(x,t)$ a generalized force.

There are several possibilities to model such a problem. Although numerical solutions, such as finite-differences, finite-element or even SPH are a popular standard, a more simple solution is here sought. In this case, we are not so much interested in computing accurately physical phenomena, such as stress or elongations within the beam, but to analyse the influence of the external loading on the beam movement, and how this modifies fluid behaviour inside the tank. Therefore, two options have been chosen. The simplest model consists on modelling the beam as a mass-spring-damper system. Therefore, Eq. (5.1) can be written as:

$$m\ddot{w} + c\dot{w} + Kw = f(t), \quad (5.2)$$

where m and c have been already defined, and K is the stiffness. This way, the solution now only depends on the temporal discretization. For a cantilever beam, the stiffness due to vertical motion takes the form $K = 3EI/L^3$. To obtain the damping, the system can be rearranged as:

$$\ddot{w} + 2\xi\omega\dot{w} + \omega^2 w = f_\omega(t), \quad (5.3)$$

where ω is the natural frequency of the system $\omega = \sqrt{K/m}$ and ξ is the damping coefficient. Identifying terms between Eqs. (5.2) and (5.3), the value of c can be established.

This solution, although simple and robust, just considers the beam as a unique spring-mass-damper system. This implies that rolling motion is not included in the model, which might be

relevant for the sloshing flow in some conditions.

Another possibility can be given according to the following expression [Rao, 2007], assuming that solution of Eq. (5.1) is a product of two functions such that:

$$w(x, t) = \phi_i(x)q_i(t), \quad (5.4)$$

which means that the problem can be split up into two different problems, one to solve the spatial discretization and another to solve the temporal evolution.

Now it is possible to substitute Eq. (5.4) into Eq. (5.1). Let's start by considering only the homogeneous solution, leaving the force term for a later analysis. Substitution yields,

$$m \phi(x) \ddot{q}(t) + c \phi(x) \dot{q}(t) + EI \phi^{IV}(x) q(t) = 0. \quad (5.5)$$

Eq. (5.5) can be split into two different problems, given by:

$$\frac{EI \phi^{IV}(x)}{m \phi(x)} = \frac{c \dot{q}(t)}{m q(t)} + \frac{\ddot{q}(t)}{q(t)} = \lambda^2. \quad (5.6)$$

This implies that the two differential equations to be solved are:

$$\phi^{IV}(x) - k_n^4 \phi(x) = 0, \quad (5.7)$$

$$\ddot{q}(t) + \frac{c}{m} \dot{q}(t) + \lambda^2 q(t) = 0, \quad (5.8)$$

where $k_n^4 = \frac{\lambda^2}{a^2}$ and $a^2 = \frac{EI}{m}$.

Regarding the spatial discretization from Eq. (5.7), we assume a solution of the form [James et al., 1994]:

$$\phi(x) = C_1 \cosh(kx) + C_2 \cos(kx) + C_3 \sinh(kx) + C_4 \sin(kx). \quad (5.9)$$

To solve this equation four boundary conditions are needed. For a cantilever beam (fixed end

Table 5.3: Solution for the first five modes of k_i and α_i .

Mode	1	2	3	4	5
k_i	1.875	4.694	7.854	10.995	14.137
α_i	0.734	1.018	0.999	1.000	0.999

at $x = 0$ and free end at $x = L$), these take the following form:

$$\begin{aligned}
 w(0, t) = X(0) = 0 \quad \frac{\partial w(0, t)}{\partial x} = \frac{\partial X(0)}{\partial x} = 0 \\
 \frac{\partial^2 w(L, t)}{\partial x^2} = \frac{\partial^2 X(L)}{\partial x^2} = 0 \quad \frac{\partial^3 w(L, t)}{\partial x^3} = \frac{\partial^3 X(L)}{\partial x^3} = 0.
 \end{aligned} \tag{5.10}$$

Applying Eq. (5.10) to the expression in Eq. (5.9), the general solution is:

$$\begin{aligned}
 \phi_i(x) &= \cosh(k_i x) - \cos(k_i x) \\
 &- \beta_i (\sinh(k_i x) - \sin(k_i x)) ,
 \end{aligned} \tag{5.11}$$

with

$$\beta_i = \frac{\cosh(k_i L) - \cos(k_i L)}{\sinh(k_i L) - \sin(k_i L)}. \tag{5.12}$$

As it has been mentioned, k_i is a function of the natural frequency. For a cantilever beam, it can be known from the solutions of the following expression:

$$\cos(k_n x) \cosh(k_n x) = -1. \tag{5.13}$$

The solution for the first five modes for k_i and α_i can be found in Table 5.3.

Eq. (5.11) is known as the normal-mode function. This function has been normalized such that:

$$\int_0^L \phi_i^2(x) dx = L \tag{5.14}$$

Applying the orthogonality properties of the normal-mode functions, as the differential equation

in Eq. (5.7) must hold for each normal mode, we can write for normal modes i and j that:

$$\begin{cases} \int_0^L \phi_i(x)\phi_j(x)dx = 0 & (i \neq j) \\ \int_0^L \phi_i(x)\phi_j(x)dx = L & (i = j) \end{cases} \quad (5.15)$$

Once the spatial solution has been found, and the eigenmodes and their corresponding natural frequencies are known, the time-dependant solution can be sought from the second equation in Eq. (5.7).

The force term can be added at this point. The general force considered in this work is a set of concentrated forces acting at determined points along the beam. A method to obtain the global force due to fluid action has been drafted in Section 3.6.1, and a sketch displaying equilibrium between fluid forces and beam reactions is illustrated in Figure 5.13.

$$f(x, t) = \sum_j^s F_j(t) \delta(x - x_j), \quad (5.16)$$

where $F_j(t)$ is the concentrated force at location j and time instant t , and x_j the corresponding location where the concentrated force is applied.

This force term added to Eq. (5.7) can be regarded as a particular solution of that homogeneous equation. Therefore,

$$f(x, t) = \frac{F}{\lambda^2} \quad (5.17)$$

is a particular solution of the homogeneous equation in Eq. (5.7).

The complete system $q(t) = q_h(t) + q_p(t)$, being $q_h(t)$ the homogeneous solution and $q_p(t)$ the particular solution respectively, is solved by means of a 4th-order Runge-Kutta algorithm in time. The total displacement at each time step can be computed from:

$$w(x, t) = \sum_i^n \phi_i(x) \cdot (q_h(t) + q_p(t)) \quad (5.18)$$

The complete system in Eq. (5.7) can now be solved and the total displacement at each time step computed. In this work, a 4th-order Runge-Kutta algorithm in time is used.

Figure 5.13: Forces equilibrium diagram. F_x , F_y and M are the forces and moment coming out from the fluid, and H , V_1 and V_2 the reactions.

5.3.3 Coupling: Results

Static test

In order to test the two beam models presented above (described according to Eqs. (5.2) and (5.18) respectively) and to set the different constants to model the beam appropriately, a static test is performed first. For this test the beam is set at rest and is loaded with different masses until a steady value of deflection is reached. Figure 5.14 presents results of both models presented in previous section versus the experimental values. Values for the models are chosen to set the same rigidity found in the experiment, meaning $E = 210 \text{ GPa}$, $I = 5.57e^{-7} \text{ m}^4$ and an effective length $L_b = 2.48 \text{ m}$. From measurements, it is found that the linear mass of the beam is $\rho_b = 13.04 \text{ kg/m}$, and therefore the total mass is 32.34 kg . As it can be appreciated, both models reproduce accurately the results from the experiment for the static test.

Dynamic Tests

Once the beam parameters are known, tests are performed.

For the dynamic tests, the tank is attached to the beam, therefore modifying the properties of the system. Two configurations for the tank are tested: a rectangular tank and a baffled tank. Geometries for both configurations can be seen in Figure 5.15. The total length of the tank is $L = 0.7 \text{ m}$ and height $H = 0.06 \text{ m}$. Baffled tank is composed by 7 compartments with length $L_i = 0.1 \text{ m}$. The total length of the tank in this case is extended to $L = 0.73 \text{ m}$, so both configurations have the same amount of fluid for a determined filling level. Filling level h can be varied, although in this work only results for filling level $h = 50\% H$ will be presented.

Figure 5.14: Displacement at the tip for the static test.

Figure 5.15: Geometry of the two configurations tested: rectangular tank (top) and baffled tank (bottom).

The beam is pre-loaded and allowed to oscillate freely, and motion, velocity and acceleration is measured. In this set of cases, the initial displacement at the tip is always the same, corresponding to $w_{tip} = 0.04\text{ m}$. In order to establish a reference, first a preliminary test without liquid is carried out. All tests carried out in this work have the same total nominal mass, which is the

corresponding to the sum of the different systems. For the solid mass test, instead of liquid, a solid mass with a weight corresponding to a 80% filling condition (the maximum tested) is attached inside the tank. Then, in the cases performed with 50% filling level, a ballast mass corresponding to the remaining mass needed, is added.

Figure 5.16 shows raw acceleration data obtained from the experiments, and those calculated with the model. Damping coefficient in the model has been set to 1.5%, which is a standard value found out in the computation of structural models, such as bridges. From this Figure it can be observed that the model response decays homogeneously, contrary to the experiment register where a more complex signal is obtained. Both results show that accelerations lie in the same order of magnitude, and that their behaviour is similar.

Figure 5.16: Acceleration registered for the modeled beam and the experimental beam for the solid mass test case without liquid.

Once the model with a solid mass is tested, some tests to compare the behaviour of sloshing fluid for the two inner configurations are shown. In the cases presented here, tank motion is

purely vertical, and no angle is induced on the tank, but the effect of fluid force on the response can be appreciated. Results for the sloshing fluid are shown in Figures 5.17 and 5.18. In

Figure 5.17: Evolution of the turbulent intensity in the fluid at five different moments of the simulation with the δ -LES-SPH model. Rectangular tank with 50% filling level.

these Figures, the evolution of the turbulent kinetic energy in log scale at five different relevant moments of the simulation are shown. Resolution in Figure 5.17 is set as $L/dr = 2000$ and in Figure 5.18 as $L_i/dr = 360$. Compact support and speed of sound are chosen the same for both tests, such that $h/dr = 2$ and $c_s = 20$ m/s. As the tank motion is purely vertical, fluid

Figure 5.18: Evolution of the turbulent intensity in the fluid at five different moments of the simulation with the δ -LES-SPH model. Baffled tank with 50% filling level.

behaviour is pretty similar at the first stages of the simulation for both tests. However, as the motion dampens, a wave is generated in the horizontal direction, and the vertical baffles play a role as they do not allow the wave to propagate. Nonetheless, there is not a noticeable influence on the turbulent kinetic energy field values.

Similarly to Figure 5.16, in Figure 5.19, accelerations registered in the experiments are compared

Figure 5.19: Acceleration registered for the modeled beam and the experimental beam for the 50% filling level baffled case.

to the numerical results obtained from the 50% filling level case for the baffled configuration. At first stages experimental data values do not match very well with numerical obtained solution, reaching values over 11 g , the maximum theoretically predicted. However, the signals tend to similar accelerations when the motion starts to dampen.

Motion damping due to fluid force is one of the key aspects to analyse in this work. In order to find a clearer comparison between the solid mass and the fluid sloshing tests regarding damping, in Figure 5.20 the non-dimensional motion time history for both the solid mass case and the fluid case obtained from the simulations is shown. As it can be seen, damping is stronger when the fluid sloshes, reaching first a stationary motion.

In Figure 5.21 this effect is emphasized. It shows the envelope of the acceleration register amplitude for the two cases presented in Figure 5.20. Damping can be obtained from the slope of the curves. At first stages, this damping is bigger for the fluid sloshing case, and then, once

Figure 5.20: Non-dimensional motion for the beam: red dashed line represents the solid mass motion, blue solid line represents the 50% fill fluid motion. $x_0 = x(t = 0)$.

the motion is sufficiently damped, both curves follow approximately the same trend, showing that fluid sloshing role loses importance and is the damping of the beam that mainly contributes to the decay in motion. This is in accordance with the fluid evolution observed in Figures 5.17 and 5.18.

Another important analysis is how the energy in the fluid evolves during the simulation. In Figure 5.22 the different energy components at the tank for the simulation with 50% filling level are shown. As it can be appreciated, in the same fashion as what is observed from previous results, there exist sharp increases in the forces and dissipation terms every time the fluid hits a wall. This can be also appreciated in variations of mechanical energy. Once motion is dampened, contributions remain stable, keeping the energy terms constant. Energy is therefore conserved.

Figure 5.21: Envelope of the acceleration register for the solid mass motion test (red dashed line) and the 50% filling fluid test (blue solid line).

5.3.4 Additional results: forces comparison with experimental data

Another interesting analysis that can be carried out from the results obtained from experiments is to show if SPH is capable of measuring forces accurately.

In order to achieve that result, the motion function obtained from the experiments for the first second of motion will be used as the input. The vertical acceleration component record is shown in Figure 5.23. Analogously, horizontal acceleration is also recorded. Both components are integrated accordingly to obtain corresponding velocities and positions.

Figure 5.24 shows the vertical force obtained in the simulations, compared to the vertical force obtained from the experiments, using the same experimental motion data. Even though the vertical force resulting from the experiment is part of a more complex motion, it is considered here as a sufficient result to show if the trends are plausible. As it can be seen, results differ considerably at the moment of the first impact. Figure 5.25 compares a detail of

Figure 5.22: Energy analysis of the vertical sloshing tank: green line represents the evolution of mechanical energy, red line corresponds to the evolution of dissipation terms, whilst blue line is the external work contribution.

Figure 5.23: Vertical acceleration record for the first second of the experiment campaign carried out at Airbus UK.

the experiment before reaching the wall and an instant of the simulation Fluid in the simulation rises as a block, hitting the top wall at the first impact. This is regarded at the forces graph in Figure 5.24 as a great short impact. Conversely, in the experiment the fluid remains attached at the bottom, and the free surface deforms in the same way as a Rayleigh-Taylor instability. Hence, forces follow motion law as the fluid moves synchronously to the tank.

Several aspects can be causing this behavior: the fact that in SPH gas phase is not being simulated, or the lack of modeling of surface tension could be possible reasons. There is, however, another aspect that influences the detachment of the liquid from the bottom and that has been largely studied in the SPH context: tensile instability. This phenomenon is occurring due to the negative pressures that appear due to the large accelerations at the first instants after the release.

In order to avoid this undesirable effect, a tensile instability correction, in the same fashion

Figure 5.24: Vertical force record for one second. Red solid line represents the experimental force. Black solid line is the obtained numerical force for the same motion.

as the one applied in Sun et al. [2017] is applied, such that the pressure gradient term F_{ij} in momentum equation (Eq. (2.16)) turns into:

$$F_{ji} = \begin{cases} p_j + p_i & p_i \geq 0 \quad \text{or} \quad i \in \mathcal{F}_s \\ p_j - p_i & p_i < 0 \quad \text{and} \quad i \notin \mathcal{F}_s. \end{cases} \quad (5.19)$$

.

Following this formulation, simulations are carried out, showing force results in Figure 5.26, where they are compared to the experimental results. As it can be seen, now SPH follows the trend, and even the secondary peaks are reproduced. There is nonetheless a gap between experimental results and SPH results that remains unveiled. Also, negative forces are captured better than positive forces. The change in behavior is emphasized in Figure 5.27, where again an instant of the experiment is compared with the numerical solution. Now, the fluid in the simulation remains attached at the bottom, and the evolution of the fluid is similar in both

Figure 5.25: Detail of the experiment at initial stages, before reaching the first maximum in acceleration after release, and same detail in the 2-D simulation.

the experiment and the simulation. This result opens a broad range of new possible analyses. Further investigations into this direction are to be carried out, including also greater resolutions, 3-D effects and additional physical models, such as surface tension.

Figure 5.26: Vertical force record for one second, with the Tensile Instability Correction (TIC) applied. Red solid line represents the experimental force. Black solid line is the obtained numerical force for the same motion.

Figure 5.27: Detail of the experiment at initial stages, before reaching the first maximum in acceleration after release, and same detail in the 2-D simulation with TIC applied.

Chapter 6

Conclusions

6.1 Summary of Thesis Achievements

This thesis provides an analysis of sloshing inside tanks within the SPH methodology. The final goal is to gain insight into the application of the method to real engineering problems.

Along the thesis, several aspects related to the numerical simulation of fluid equations within a confined domain have been analyzed. In particular, these aspects focus on the formulation of the boundary conditions, which are a critical aspect in SPH that is still not fully understood, being indeed selected as one of the Grand Challenges that the SPH community has to further investigate in the upcoming years. The different boundary conditions formulations that have been developed and are available in the literature have been reviewed, showing similarities and differences between them, and finally classifying them in two groups: fluid extensions and contour closure techniques. The latter are a relatively novel approach that arise as a combination of two primitive methodologies. Their potential for future applications is huge, but several shortcomings have still to be studied. One of these problems is related to the truncation of kernel radius at the boundary. A novel solution is proposed in this thesis, based on the transformation of the volume integral used for the computation of the Shepard renormalization factor into a surface integral, hence integrating naturally the concept of boundary within the SPH framework and allowing for a geometrical computation that permits a more accurate solution. Results shown for a hydrostatic case, which is always a real challenge in SPH, and a

3-D dam-break illustrate the potential of the method to solve impact problems and in general sloshing inside tanks.

Additionally, conservation properties within the boundary integrals formulation are studied. Based on the properties of volume integrals used solely in fluid extensions, a link to the boundary integrals methodology has been established through generalized surface local coordinates. This general formulation is then applied to the forces computation, that improves current formulation, as it allows to compute forces along partial boundaries within the domain, and additionally keeps momentum conservation.

Consistency of energy balance equation is also studied in a boundary integrals context, extending preliminary analysis that can be barely found in the literature [Cercos-Pita et al., 2017].

These two analysis are tested through an application case, in which a square is moved inside a fluid box. Results show that the methodology preserves momentum and that is consistent regarding energy balance.

Additional features that have been found interesting aspects to improve SPH capabilities to deal with sloshing flows are implemented in a fully free SPH software, namely AQUA_{gpusph}. In particular, Particle Packing algorithm presented by Colagrossi et al. [2012] for fluid extension methodology, is extended to the boundary integrals methodology. Also, a free surface particle tracking algorithm, based on previous formulations by Marrone et al. [2010] and Sun et al. [2019a] is implemented.

Two novel methodologies are also implemented. Navier-Stokes equations, revisited from a LES perspective by Di Mascio et al. [2017], are implemented, so that simulations at moderate and high Reynolds numbers can be carried out. Additionally, diffusive coefficients, both in continuity and momentum equations, are now implicitly included in the formulation, having both physical meaning, and hence, no tuning of parameters is needed. Moreover, a single-phase phase change model is derived and implemented within the code, based on the fact that the gas phase role in the flow can be modeled assuming homogeneous values for the thermodynamic variables, and hence, only interacts with the liquid phase, that is explicitly solved, through the interface at the free surface.

Finally, several application cases are presented. With the 3-D dam-break capabilities of the novel formulation regarding boundary treatment are outlined, showing that it is able to deal with impact flows in the same way as other currently used methodologies. Also, 3-D simulations of moving containers can be satisfactorily carried out. In particular, an anti-roll tank with baffles is simulated at different frequencies and compared to experimental data, showing reasonable agreement with them.

A vertical sloshing of a fully coupled fluid-structure interaction problem is also simulated, in order to analyze additional damping induced by fluid in aircraft wings. In order to reproduce experimental results, the fluid is simulated with the δ -LES-SPH model, whilst the structure is based on standard beam theory. From the results, it can be concluded that SPH is able to confirm that the presence of liquid inside a tank attached to a flexible structure induces a damping that can be measured in terms of motion. Also, that SPH is able to deal with complex baffled geometries.

To sum up, in order to improve SPH capabilities regarding the simulation of sloshing flows, three main topics are discussed in this work: first, theoretical aspects, involving boundary integrals methodology and conservation properties, are analyzed. Two novel formulations are derived to reduce inconsistencies at the free surface in the presence of solid boundaries and allow for a correct computation of forces. Second, a set of useful tools and physical models are implemented into AQUA_{gpusph}. Both tools and models can be used to improve the physics involved in sloshing. Third, studies on relevant application cases are carried out, including 3-D geometries, an anti-roll tank, and a vertical sloshing test case.

6.2 Future Work

There are additional aspects that are left open for future consideration that extend far beyond the analysis carried out in this work. In particular, the author has identified several, who are outlined below for the various reasons documented:

1. The formulation introduced for the boundary integrals technique has been carried out for a particular kernel. It would be interesting to extend this analysis to other kernels widely

used in the literature, such as C4 and C6 Wendland kernels, and investigate which is the role of the kernel function on the SPH solution, in a similar fashion to what has been done in 1-D for a hydrostatic case by Merino-Alonso et al. [2019].

2. Aspects related to adaptivity, including particle split-coalesce algorithms and shifting, have been here left for future analysis. However, they seem a promising approach in order to deal with large simulations on one hand, in which adaptive resolution can play a significant role in performance, and a regular lattice of particles on the other hand. Shifting in the presence of a free-surface has been identified as a challenge, especially due to the fact that is difficult to keep volume unchanged [Michel et al., 2018]. A consistent approach to shifting has been presented in Sun et al. [2019a], that needs further analysis.
3. As δ -LES-SPH methodology is a relatively new tool, there are a few aspects that need to be still further analyzed. In particular, identification of constants and parameters, and an analysis of their influence on the solution, is needed. There is also the question on how to deal with these parameters in the presence of solid boundaries, and how the diffusive terms associated to α_i and δ_i parameters behave when velocities do not play a significant role, as both values depend on the velocity gradients.
4. Modeling phase change for sloshing in cryogenic conditions has been identified as a key aspect that has received little attention from the research community and has a range of potential future applications. Moreover, phase change for liquid-gas mixtures has not been reported before as far as the author is concerned. In this thesis, a novel perspective is presented, where the emphasis is put only on the mass exchanges through the interface between the fluid phases involved. Despite the potential shown, more work is necessary to be done. Particularly, when moving to more complex geometries, the model is not able to represent accurately variations of mass instantaneously, as they depend on particle size. The application of a particle split-coalesce algorithm and variable resolution at the interface might be a possible solution to improve this aspect that needs to be further studied.
5. Additional models and methodologies can be implemented in order to improve sloshing

assessment with AQUA_{gpusph}. A multiphase approach might help in the determination of the air phase in certain aspects and situations in which air entrapment has been identified as a mechanism affecting sloshing. It has also been seen in the present work that the presence of air can have a significant role on the pressure impact at the wall, and this has been also previously studied in FVM contexts Braeunig et al. [2009]. A δ -SPH model for multiphase flows has recently been presented by Sun et al. [2019b].

Phase change analysis can also benefit from the secondary phase, despite the penalties associated to performance and computational cost. Phase change considering dynamics of both phases is currently a topic that is deserving attention from research community [Behruzi and Konopka, 2015, Ancellin et al., 2018]

Surface tension models can also be relevant in certain situations, such as cryogenic sloshing, in which inertial forces associated to gravity become residual. A surface tension model can be derived from the free surface particle tracking technique used in this thesis, analogous to Morris [2000].

6. Regarding coupling between fluid and structural solvers, there are still efforts to be made in several directions. Models are limited to 1-D, for the case of the mass-spring-damper system, and 2-D for the modal solution. More degrees of freedom can be added in order to set accurately the motions in complex situations. From the fluid perspective there is still a need for further refinement in order to capture as much turbulent phenomena as possible. The particular characteristics of the flow and the greatly violent motion induced to the tank, makes it necessary to carry out further research into tensile instability and anti-clumping corrections, in order to reach stable and reliable simulations. 3-D effects need to be investigated as they may play a role in the damping mechanisms, especially when inner baffled configurations are introduced. Also energy transfer mechanisms between both systems are to be explored.

Papers written during the PhD studies

Journal papers

Pérez-Arribas, F and Calderon-Sanchez, J (2020). A parametric methodology for the preliminary design of SWATH hulls. *Ocean Engineering*, 197, 106823.

Calderon-Sanchez, J., Cercos-Pita, J. L., & Duque, D. (2019). A geometric formulation of the Shepard renormalization factor. *Computers & Fluids*, 183, 16-27.

Calderon-Sanchez, J., Duque, D. & Gómez-Goñi, J. (2015). Modeling the impact pressure of a free falling liquid block with OpenFOAM. *Ocean Engineering*, 103, 144-152.

Conference papers

In bold, the papers presented by the candidate.

Calderon-Sanchez, J., González, L.M., Marrone, S., Colagrossi, A., Gambioli, F. A SPH simulation of the sloshing phenomenon inside fuel tanks of the aircraft wings (2019). In *14th International SPHERIC Workshop*, Exeter, United Kingdom.

Calderon-Sanchez, J., Duque, D., & Gómez-Goñi (2018, June). Modeling the Effect of Phase Change on LNG Impact With Open-Source CFD. In *ASME 2018 37th International Conference on Ocean, Offshore and Arctic Engineering*. American Society of Mechanical Engineers Digital Collection.

Bernal-Colio, V. R., Cercos-Pita, J. L., Calderon-Sanchez, J., Diaz-Ojeda, H. R., Abad, R., & Souto-Iglesias, A. (2018, June). Numerical Modeling of the Forced Motion Dynamics of Antiroll Tank With OpenFOAM. In *ASME 2018 37th International Conference on Ocean, Offshore and Arctic Engineering*. American Society of Mechanical Engineers Digital Collection.

Calderon-Sanchez, J. Cercos-Pita, J. L., Duque, D. A new Shepard renormalization factor formulation for Boundary Integrals (2018). In *13th International SPHERIC Workshop*, Galway, Ireland.

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Cercos-Pita, J.L. , Zisis, I. , Messahel, R. , & Calderon-Sanchez, J. AQUAgpusph: The SPH of the researchers, by the researchers, to the researchers. (2017) In *12th International SPHERIC Workshop*, Ourense, Spain.

Calderon-Sanchez, J., Duque, D., Souto-Iglesias, A. A single-phase SPH model for evaporation and condensation phenomena (2017) In *12th International SPHERIC Workshop*, Ourense, Spain.

Appendix A

Detailed derivations for the kernel expressions

A.1 Expressions for the divergent part of F

It is worth mentioning that the expressions for the divergent part of F (F_D), i.e. the last terms in Eqs. (3.24, 3.25) are not limited to a particular kernel choice. Indeed, by its definition in Eq. (3.22), F is found by solving

$$[\mathbf{r}'^d F(\mathbf{r}')]_{\mathbf{r}^d F(\mathbf{r})}^0 = \int_{\mathbf{r}}^{sh} \mathbf{r}'^{d-1} W_h(\mathbf{r}') d\mathbf{r}', \quad (\text{A.1})$$

where the integration limits guarantee that F will have the same support as W_h .

If we consider the $\mathbf{r} \rightarrow 0$ limit, this yields

$$-\mathbf{r}^d F_D(\mathbf{r}) = \int_0^{sh} \mathbf{r}'^{d-1} W_h(\mathbf{r}') d\mathbf{r}'. \quad (\text{A.2})$$

But, due to the kernel normalization, the right-hand side integral is $1/2\pi$ in 2-D, or $1/4\pi$ in 3-D. From this fact, the same expressions for F_D will arise in general. Notice that $\mathbf{r} F_D(\mathbf{r})$ is basically the Coulomb field of a point particle, hence what is derived here closely follows the demonstration of Gauss' Law in electrostatics.

Figure A.1: Sketches of the integration over patches in 2-D (left) and 3-D (right).

In Figure A.1 (left) the 2-D situation is sketched for a generic patch (index “ j ” will be dropped, for the sake of readability). The distance $\mathbf{y} - \mathbf{x}$ can be decomposed in a constant normal distance to the patch (r_n), and a component tangent to the wall (r_t), which is the integration variable.

The integrals that appear in (3.27) are of the form

$$\mathbf{n} \cdot (\mathbf{y}_j - \mathbf{x}) \int_S F(\mathbf{y} - \mathbf{x}) d\mathbf{y} = r_n \int_S F(\mathbf{r}) dr_t = -\frac{r_n}{2\pi} \int_S \frac{1}{r^2} dr_t. \quad (\text{A.3})$$

It is straightforward to demonstrate this equality,

$$\frac{r_n}{r^2} dr_t = d\theta, \quad (\text{A.4})$$

(an expression which also appears in the calculations of the electrostatic field of a charged thin rod) from which Eq. (3.28) results.

Figure A.1 (right) sketches the 3-D situation. In this case, the integrals have this form

$$\mathbf{n} \cdot (\mathbf{y}_j - \mathbf{x}) \int_S F(\mathbf{y} - \mathbf{x}) d\mathbf{y} = r_n \int_S F(\mathbf{r}) dS = -\frac{r_n}{4\pi} \int_S \frac{1}{r^3} dr_t. \quad (\text{A.5})$$

In the same manner, we may demonstrate

$$\frac{r_n}{r^3} dS = d\Omega, \quad (\text{A.6})$$

this is, the differential of a solid angle. This way, Eq. (3.29) is obtained.

A.2 Efficient evaluation of the angle subtended by a patch

As discussed above, the alternative Shepard renormalization factor boils down to the computation of a convolution boundary term and an angle subtended by a boundary patch. The former convolution boundary term, associated to the non-singular part of kernels in Eqs. (3.24, 3.25), can be in fact computed applying the boundary integrals approach described by Ferrand et al. [2013] and Cercos-Pita [2013]. However, this is clearly not the case of the angle subtended by boundary patches.

As the boundary integrals methodology itself, the angle subtended by a boundary patch computation admits both a semi-analytical approach [Ferrand et al., 2013] and a purely numerical one [Cercos-Pita, 2013], being the latter more efficient but less precise than the former. Both approaches will be discussed here, in order to highlight their similarities and differences.

A.2.1 Semi-analytical methodology

When the semi-analytical boundary integrals methodology is applied, as described by Ferrand et al. [2013], the boundary is discretized in planar patches, each defined by its vertices and normal vector, as it is schematically depicted in Fig. A.2.

Indeed, in 2-D simulations the boundary is discretized in line segments, such that the tangent distance of a generic j^{th} vertex,

$$r_j^t = |(\mathbf{y}_j - \mathbf{x}) - \mathbf{n}_j (\mathbf{n}_j \cdot (\mathbf{y}_j - \mathbf{x}))|, \quad (\text{A.7})$$

can be used to compute the angle subtended by the generic j^{th} line segment:

$$\Delta\theta_j = \tan^{-1} \left(\frac{r_{j+1}^t}{r^n} \right) + s_t \tan^{-1} \left(\frac{r_j^t}{r^n} \right), \quad (\text{A.8})$$

Figure A.2: Schematic view of the subtended angle computation within the semi-analytical context Ferrand et al. [2013].

with

$$s_t = \text{sign} \left(|\mathbf{y}_j - \mathbf{x}| - (r_{j+1}^t - r_j^t) \right). \quad (\text{A.9})$$

Even though 3-D boundaries can be discretized by a wide variety of planar patches, only triangulations will be discussed here. The expression to compute angles subtended by triangular plates, discussed in Van Oosterom and Strackee [1983], can be applied:

$$\begin{cases} \mathbf{a} = \mathbf{y}_j - \mathbf{x}, \\ \mathbf{b} = \mathbf{y}_{j+1} - \mathbf{x}, \\ \mathbf{c} = \mathbf{y}_{j+2} - \mathbf{x}, \\ \Delta\Omega_j = \frac{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}{abc + a(\mathbf{b} \cdot \mathbf{c}) + b(\mathbf{a} \cdot \mathbf{c}) + c(\mathbf{a} \cdot \mathbf{b})} \end{cases} \quad (\text{A.10})$$

A.2.2 Purely numerical methodology

In the purely numerical boundary integrals methodology (details of the implementation can be found in Refs. Cercos-Pita [2013, 2015]), the same discretization applied to the volume particle is naturally extended to the boundary, i.e. the boundary is sampled by boundary elements associated to a boundary area portion. Indeed, mesh connectivity between elements is not required any more, which permits a substantial improvement of computational performance. On the other hand, truncation errors are introduced, meaning lower quality results.

In fact, the 2-D implementation is rather similar to the semi-analytical one, discussed in A.2.1.

Figure A.3: Schematic view of the subtended angle computation within the purely numerical context Cercos-Pita [2013].

The boundary is discretized in line segments that, in contrast to the semi-analytical approach, are defined by their center $\mathbf{y}_j$, area S_j and normal $\mathbf{n}_j$, as schematically depicted in Fig. A.3 (left). Analogously, we can compute the tangential distance to the generic j^{th} boundary element center,

$$r_j^t = |(\mathbf{y}_j - \mathbf{x}) - \mathbf{n}_j (\mathbf{n}_j \cdot (\mathbf{y}_j - \mathbf{x}))|, \quad (\text{A.11})$$

with an expression for the angle subtended by the boundary element similar to the one already found for the semi-analytical methodology,

$$\Delta\theta_j = \tan^{-1} \left(\frac{r_j^t + S_j/2}{r^n} \right) - \tan^{-1} \left(\frac{r_j^t - S_j/2}{r^n} \right). \quad (\text{A.12})$$

The 3-D case is much more complex. The boundary is then discretized in square area elements, defined by their center $\mathbf{y}_j$, area S_j , normal $\mathbf{n}_j$ as schematically depicted in Fig. A.3 (right). A tangent vector $\mathbf{t}_j$ is considered, whose choice does not affect the results, as long as it is contained in the plane of the square. To compute the solid angle subtended by the boundary element we can make use of the well known expression of the solid angle subtended by a rectangular patch in which one corner coincides with the projection of the origin, $\mathbf{x}$, onto the plane:

$$\Omega(a, b, r^n) = \cos^{-1} \left(\sqrt{\frac{1 + (a/r^n)^2 + (b/r^n)^2}{(1 + (a/r^n)^2)(1 + (b/r^n)^2)}} \right), \quad (\text{A.13})$$

with a and b being the width and height of the rectangular patch respectively.

To this end, we can compute the tangential distances,

$$\begin{aligned} r_j^t &= |\mathbf{t}_j \cdot (\mathbf{y}_j - \mathbf{x})|, \\ r_j^b &= |\mathbf{b}_j \cdot (\mathbf{y}_j - \mathbf{x})|, \end{aligned} \tag{A.14}$$

where $\mathbf{b}_j$ is the binormal vector, $\mathbf{n}_j \times \mathbf{t}_j$. The subtended solid angle is subsequently computed as follows:

$$\begin{aligned} \Delta\Omega_j &= \Omega\left(r_j^t + \frac{\sqrt{S_j}}{2}, r_j^b + \frac{\sqrt{S_j}}{2}, r^n\right) \\ &\quad - s_t \Omega\left(r_j^t - \frac{\sqrt{S_j}}{2}, r_j^b + \frac{\sqrt{S_j}}{2}, r^n\right) \\ &\quad - s_b \Omega\left(r_j^t + \frac{\sqrt{S_j}}{2}, r_j^b - \frac{\sqrt{S_j}}{2}, r^n\right) \\ &\quad + s_t s_b \Omega\left(r_j^t - \frac{\sqrt{S_j}}{2}, r_j^b - \frac{\sqrt{S_j}}{2}, r^n\right), \end{aligned} \tag{A.15}$$

with

$$\begin{aligned} s_t &= \text{sign}\left(r_j^t - \frac{\sqrt{S_j}}{2}\right), \\ s_b &= \text{sign}\left(r_j^b - \frac{\sqrt{S_j}}{2}\right). \end{aligned} \tag{A.16}$$

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