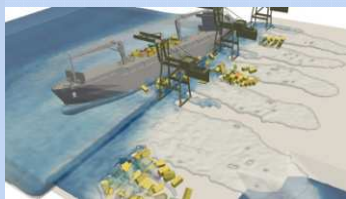
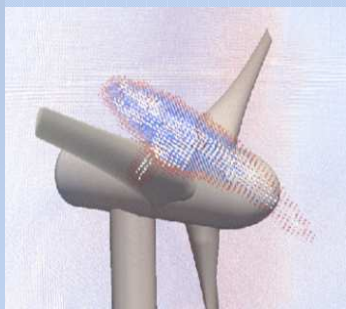
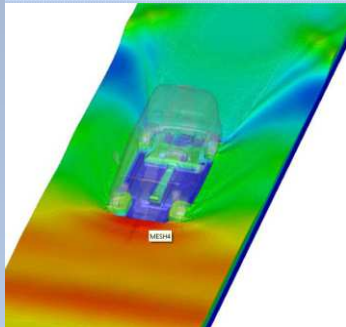
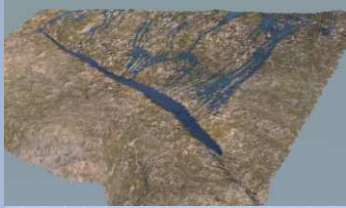


Proceedings of the  
**9<sup>th</sup> SPHERIC**  
**International Workshop**  
3–5 June 2014, Paris



*D. Violeau  
A. Hérault  
A. Joly*  
**editors**



**le cnam**



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May 2014

## Foreword to the 9<sup>th</sup> SPHERIC International Workshop

Dear delegate,

The Research and Development division of Electricité de France, the Conservatoire National des Arts et Métiers and The Saint-Venant Laboratory for Hydraulics are delighted to host the 9<sup>th</sup> SPHERIC International Workshop.

Since SPHERIC was born in 2005, the annual International Workshop has been the central event of our community, with exciting scientific talks and fruitful discussions. This is the place for all SPH researchers, students and practitioners to share knowledge and present their improvements, in a stimulating and friendly atmosphere. The present workshop in Paris will be of particular interest with the recent creation of the Grand Challenge Working Group, while SPHERIC is approaching its tenth anniversary.

This workshop received 83 abstracts of good quality, and 60 of them were selected to appear in the present proceedings. This demonstrates the success of SPHERIC in fields ranging from sediment transport, solid mechanics and astrophysics to heterogeneous High Performance Computing and GPU programming. The present proceedings will allow the participants to enjoy a comprehensive description of the work exhibited by the speakers.

For the 9<sup>th</sup> SPHERIC International Workshop, it is with great pleasure that we welcome you all to the City of Paris.

Thank you for your participation.

Two handwritten signatures in black ink. The first signature is on the left, appearing to be 'D. Violeau', and the second is on the right, appearing to be 'A. Hérault'.



Damien Violeau, EDF  
Alexis Hérault, CNAM  
Chair of the Local Organising Committee

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# A Multi-Phase Particle Shifting Algorithm for SPH Simulations for Violent Hydrodynamics on a GPU

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**Abstract**—This paper investigates the use of a shifting algorithm for improving the results of smoothed particle hydrodynamics (SPH) multi-phase simulations by preventing the creation of unnatural voids. Particle shifting occurs according to a Fickian-based algorithm so particles maintain a nearly uniform distribution. A modification of the shifting algorithm is necessary in the air phase to avoid unphysical void formation. In conjunction with the use of graphics processing units (GPUs) for the acceleration of the simulation, the new shifting algorithm allows the simulation of complex multi-phase flows such as a wet dam break and a sloshing tank. Finally, the shifting algorithm is extended to 3-D and validated with the SPHERIC benchmark test case of dam break impacting an obstacle.

## I. INTRODUCTION

Multi-phase flows with mixing and violent free-surface hydrodynamic interaction, a common sight in both industrial and natural phenomena, are an ideal application of smoothed particle hydrodynamics (SPH). A diverse range of problems such as overturning or breaking waves and potentially explosive multi-phase pipe flow require accurate multi-phase simulations with a large number of particles due to the constantly changing free-surface making the interface between the fluids the most important and challenging aspect.

Including multiple phases in SPH is relatively straightforward, as it is possible to assign a separate set of particles to each phase [1]. Handling the interactions among them however, is greatly dependent on their physical and hydrodynamic properties such as density. Treatment of the interface may be necessary. A number of multi-phase SPH models have already been developed addressing such issues [2].

SPH is a modelling method with extremely high computing requirements due to the integral interpolation and its simulations require a substantial time period. This drawback is particularly important when simulating multi-phase flows as a larger domain and a greater number of particles is required. The interactions at the interface and the different qualities of the fluids may also necessitate a smaller time step and a finer resolution.

To reduce the computational runtimes, the use of graphics processing units (GPUs) has been proposed [3]. Their massively parallel architecture is an ideal fit for the Lagrangian methods used in this study enabling the modelling of finer resolutions and very large numbers of particles. Accelerating the simulation with a GPU gives significant

speedups for even just one graphics card over the equivalent conventional CPU codes for simulations of 10-20 million particles [4]. It has already been used for accelerating multi-phase flows with significant speed-ups recorded against a conventional CPU code [5].

The higher resolutions possible with GPUs have now highlighted a number of problems when applied to multi-phase SPH simulations which persist regardless of the resolution used. The creation of unphysical voids is a major one, especially in entrained flows. Smaller voids can also be created for water particles suspended in the air phase. The objective of this paper is, then, to present a treatment to these issues allowing the simulation of complex multi-phase flows with millions of particles.

Particle shifting techniques have recently emerged as an attractive additional operation to avoid unphysical and numerically unstable particle arrangements. The use of a shifting algorithm, initially presented within a divergence-free incompressible SPH approach [6] is proposed to prevent the instability caused by anisotropic particle spacing. The algorithm was improved by Lind et al. who proposed a free-surface correction to the Fickian-based algorithm to ensure that the particle positions maintain an approximately uniform particle distribution [7] and further by Skillen et al.[8] who improved the calculation of the diffusion term.

In this paper, the shifting algorithm has been further modified in order to apply to a weakly compressible multi-phase SPH approach instead of a fully incompressible model. An investigation has also been performed regarding the effect of the free-surface correction. This work shows that altering the shifting algorithm is necessary in the air phase where voids can occur near the surface and are prevented through greater Fickian motion by simply switching off the surface correction in the air phase. The results are demonstrated using the overturning wave on a dam break case. Validation of the results is also performed with different cases including a dam break on a wet bed [9] and a sloshing tank case. The shifting algorithm has also been expanded to 3-D space with results presented for a wave impact case [10].

The structure of this paper is as follows: first we present the governing equations and SPH discretisation used on the GPUs. The next section presents the shifting algorithm as described by Lind et al. [7] and Skillen et al.[8] as well as the DualSPHysics code [11]. The issues encountered in high resolutions are further elaborated and the modifications of the

# 3-D SPH Modelling of Sediment Scouring Induced by Rapid Flows

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**Abstract**—In this paper, a novel two-phase SPH scheme is developed to model scour of non-cohesive sediment suspension. To model the sediment scour due to intense fluid flows the Drucker-Prager yield criterion has been used to evaluate the yielded region of the sediment. The dynamics of the yielded region are modelled using the Herschel-Bulkley-Papanastasiou viscoplastic model for low and high stress states with a variable yield stress calculated by the sediment skeleton pressure. Also, the seepage force exerted on the sediment is included in the governing equations. Finally, the suspension of the saturated sediment particles is modelled using a statistical colloidal model based on the volumetric concentration. The model has been validated using a well-known 3-D dam break test case with close agreement to the experimental data. The multi-phase model is implemented in DualSPHysics using Graphic Processing Units (GPUs) to accelerate the computations with satisfactory speeds.

## I. INTRODUCTION

Problems that involve two or more phases, highly non-linear deformations and free-surface flows are a common occurrence in applied hydrodynamic problems. Sediment resuspension and scouring at the bottom of industrial tanks is used widely for mixing, filtration, heat generating sediment flows and reservoir scouring.

A real life engineering application is being developed for the UK nuclear power industry where the resuspended sediment is agitated in industrial tanks by rapidly-varying flows with internal jets. The current application is very difficult to treat with traditional CFD approaches due to the fluid-sediment interface, the highly non-linear deformation of the sediment and particle entrainment of the sediment particles by the fluid phase with additional heat effects. This makes the problem ideal for SPH development on graphics processing units (GPUs) to enable simulation of real engineering problems with a large number of particles.

These subaqueous sediment scouring flows are induced by rapid inflow creating shear forces at the surface of the sediment which yield the surface and produce a shear layer of suspended particles at the interface and finally sediment suspension in the fluid. Resolving small-scale effects at the interface is essential to capturing complex industrial flows accurately with variable physical properties for each phase. The massively parallel architecture of GPU computing can dramatically accelerate

simulations to simulate fine particle resolutions required for such industrial applications in realistic time.

In this paper, a multi-phase fluid-sediment model based on a yield criterion and a constitutive viscoplastic equation together with sub-closure models such as the seepage force has been implemented in DualSPHysics [1] to model the scour and sediment suspension at the interface with attention to the viscous forces of the yield and suspended sediment particles.

The paper is organized as follows; Section II.A describes briefly the fluid model whereas II.B presents the sediment model in detail. Section III describes the GPU implementation followed by the results and conclusions.

## II. NUMERICAL MODEL

In this section, the governing equations and the modelling technique for the fluid and sediment phase are presented. Throughout this paper, superscripts  $\alpha$  and  $\beta$  denote the Cartesian coordinates using Einstein's summation and  $i$  and  $j$  the interpolated particle and its neighbours respectively.

### A. Governing equations

The governing equations for density and momentum evolution of the field for the multi-phase model are given by [2]

$$\left\{ \begin{array}{l} \frac{d\rho_i}{dt} = \rho_i \sum_j^N \frac{m_j}{\rho_j} u_{ij}^\beta \frac{\partial W_{ij}}{\partial x_i^\beta} \\ \frac{du_i^\alpha}{dt} = \sum_j^N m_j \left( \frac{\sigma_i^{\alpha\beta} + \sigma_j^{\alpha\beta}}{\rho_i \rho_j} \right) \frac{\partial W_{ij}}{\partial x_i^\beta} + g_i^\alpha, \\ \frac{dx_i^\alpha}{dt} = u_i^\alpha \end{array} \right. \quad (1)$$

where  $x_i^\alpha$  is the position,  $u_i^\alpha$  is the velocity,  $\rho$  is the density,  $\sigma_i^{\alpha\beta}$  is the total stress tensor,  $m$  is the mass and  $g_i^\alpha$  is the gravitational force. The total stress tensor  $\sigma_i^{\alpha\beta}$  is made up from the isotropic pressure  $p_i$  and the viscous stresses according to

$$\sigma_i^{\alpha\beta} = -p_i \delta^{\alpha\beta} + \tau_i^{\alpha\beta}, \quad (2)$$

where the viscous stresses are

# SPH modelling of granular flows

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**Abstract—** This study describes the development of a 2-phase 3D SPH model for granular flows. The numerical solution is based on a SPH approximation of the mixture model of Chauchat-Médale (2010), a 2D finite volume code. The new model represents the dynamics of a mixture of pure fluid (e.g. water) and solid granular material (e.g. sand; mixture viscosity is not a tuning parameter).

Further, we have investigated a faster and approximated solution, in case erosion is the only cause of mobilization for solid grains.

Preliminary validations involve three 2D erosional dam breaks, a 2D submerged landslide and a 3D erosional dam break. Further, we provide model inter-comparisons on a 2D flushing test case and represent a demonstrative 3D dam breach event.

## I. INTRODUCTION

Numerical modelling of granular flows interest several application fields: erosion and bed-load transport phenomena, sediment removal in water reservoirs (flushing), erosional dam breaks, dam breaches (earth-filled dams), fast landslides.

SPH technique ([21],[28],[25]) has been already applied to granular flows in 2D ([17], 2D erosion criterion) and for several studies on 2D landslides (e.g. [3]). In general, the reference (mesh-based or mesh-less) CFD models for granular flows are 2D (mainly with the Shallow Water approximation), usually need ad-hoc tuning for the granular mixture viscosity and can be applied to a limited number of phenomena.

In this context, we have developed a 3D 2-phase SPH model for granular flows. The numerical solution is based on a SPH approximation of the mixture model of [4], a 2D finite volume code. The new model represents the dynamics of a mixture: pure fluid (e.g. water) and solid granular material (e.g. sand). In this model mixture viscosity is physically estimated (i.e. it is not a tuning parameter).

Further, we have investigated a faster and approximated solution, in case erosion can be considered the only cause of mobilization for solid grains. Under this condition, we can avoid modelling the whole granular material and treat only the eroded particles. In this frame, we have used the 2D erosion scheme of [17] and modified it implementing two main features: the coefficient for generic 3D bed slope inclination of [30] and an algorithm to allow the mixture (not only the pure fluid) to erode the fixed bed.

After this introduction, we describe the numerical model (Sec.II), the results of this study and conclusions (Secs.III,IV).

## II. THE NUMERICAL MODEL

This section describes the main features of the numerical model (Sec.II.A.) and the erosion scheme which can be eventually activated to speed-up the code (Secs.II.B,II.C.). A complete description of the model is available in [2].

### A. Governing equations of a 3D 2-phase SPH model for granular flows

The 3D 2-phase SPH model is based on the governing equations of [4], here adapted to SPH formalism.

Let first refer to the definition of the mixture density  $\rho$  (subscript “m” for mixture can be omitted hereafter):

$$\rho = (1 - \phi_f)\rho_f + \phi_s\rho_s \quad (1)$$

where  $\phi$  is the volume fraction, and the subscripts “f” and “s” refer to the fluid and solid phase, respectively.

We use the continuity equation derived in [4], adapted to a Weakly-Compressible (WC) approach:

$$\frac{d\rho}{dt} = -\rho \frac{\partial u_j}{\partial x_j} \quad (2)$$

where  $\rho$  is density,  $\underline{u}$  is velocity and Einstein notation works for the subscript “j”.

We then adopt the following continuity equation using the boundary scheme of [6]:

$$\begin{aligned} \frac{d\rho_0}{dt} = & \rho_0 \sum_b (u_{b,j} - u_{0,j}) \frac{\partial W}{\partial x_j} \Big|_b \omega_b + \\ & + 2\rho_0 \int_{V_h} [(u_w - u_0) \cdot \underline{n}] n_j \frac{\partial W}{\partial x_j} dx^3 \end{aligned} \quad (3)$$

The subscripts “0”, “b” and “w” refer to the computational particle, its neighbouring particles and frontiers, respectively.  $W$  represents the kernel function,  $\underline{n}$  the frontier normal vector,  $\omega$  is the particle volume.

The reference momentum equation ([4]) is:

$$\frac{du_i}{dt} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} - \delta_{ij} g + \nu_m \frac{\partial^2 u_i}{\partial x_j^2}, \quad \nu_m = \frac{\mu_m}{\rho} \quad (4)$$

where  $\nu_m$  is the mixture kinematic viscosity,  $g$  gravity,  $p$  pressure and Einstein notation works for the subscript “j”.

The mixture dynamic viscosity takes the form:

$$\mu_m = \frac{\phi}{\phi_{max}} \frac{\sigma'_{stan\phi}}{\lambda_* + \sqrt{I_2(e_{ij})}} + \mu_e, \quad \lambda_* = 1.0 * 10^{-4} s^{-1} \quad (5)$$

# Two-phase benchmarks for SPH multiphase fully compressible schemes

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**Abstract**—SPH schemes for multiphase simulations in the fully compressible regime are studied with four one-dimensional test cases. They come from a well-studied variational SPH framework and incorporate artificial diffusion coming from a generic formula. It is shown that this standard approach for SPH may treat multiphase processes in the fully compressible regime, without reverting to non-standard formulations. Results are compared to results from the Arbitrary Lagrangian Eulerian method and validated against exact solutions.

## I. INTRODUCTION

Multiphase problems in SPH have received substantial attention, due to SPH's straightforward way of introducing more than one fluids in the computational domain [1]. Especially for the weakly compressible regime, multiphase algorithms have been extensively studied [1]–[6] and remedies have been pinpointed and often fixed. Validated results have been reported involving density ratios of 1,000, by simply using standard SPH algorithms [6].

In all these schemes, it is common practice to use particles of different masses for each phase, such that particle mass ratios correspond to the initial density ratios. However, for the simulation of processes in the fully compressible regime, particles of equal masses are advised [7]. For such systems, the ratio of initial spacings between particles of each phase is the ratio of the densities. Thus, the spacing of particles in the lowest-density region regulates the discretization length and hence the number of particles in the system. Therefore, simulations involving high density ratios—like air-water shock tubes—are either computationally implausible or are bound to be coarse.

SPH has been frequently criticized for its ability to simulate multiphase processes (for this discussion see [8], [9]) and alternative formulations have appeared [10], [11], where particle volumes are obtained from thermodynamics rather than density. However, the standard framework, as reviewed by Monaghan [1] and [9], is better studied, offers a well-established spatial adaptivity and provides a generic formula for artificial dissipative terms.

The aim of the present article is to show that the SPH standard framework is able to treat multiphase problems, when

equipped with particles of unequal masses and the differential form of mass conservation. Unless one is interested in building higher order schemes for density, computing the latter is more popular for open domains and more robust than using the integral form [5]. These four benchmarks involve one-dimensional shock tubes with discontinuous initial data and discontinuous fluid parameters, as well. In order to show that SPH results are comparable to the results obtained by more advanced numerical techniques, problems are also solved with the Arbitrary Lagrangian-Eulerian (ALE) method, which utilizes fluid mixing theory. Finally, results are validated against exact solutions.

## II. EQUATIONS

Considering both integral and differential forms of mass conservation, two popular density estimates deliver four SPH schemes, after casting them into the SPH variational framework of [1], [9]. The integral form of the traditional approach is:

$$\langle \rho_i \rangle := \sum_j m_j W_{ij, h_i}, \quad h_i := \eta \left( \frac{m_i}{\rho_i} \right)^{\frac{1}{n}}, \quad (1)$$

or its differential counterpart:

$$\frac{d\langle \rho_i \rangle}{dt} = \frac{1}{\Omega_i} \sum_j m_j (\mathbf{v}_i - \mathbf{v}_j) \nabla_i W_{ij, h_i},$$

$$\Omega_i = 1 - \frac{\partial h_i}{\partial \rho_i} \sum_j m_j \frac{\partial W_{ij}}{\partial h_i}, \quad h_i = \eta \left( \frac{m_i}{\rho_i} \right)^{1/n}, \quad (2)$$

deliver their corresponding equation of motion for each particle:

$$\frac{d\mathbf{v}_i}{dt} = - \sum_j m_j \left( \frac{P_i}{\langle \rho_i \rangle^2 \Omega_i} \nabla_i W_{ij}(h_i) + \frac{P_j}{\langle \rho_j \rangle^2 \Omega_j} \nabla_i W_{ij}(h_j) \right), \quad (3)$$

# A non-Newtonian ISPH scheme for improved prediction of pressure fields

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**Abstract**—A new incompressible smoothed particle hydrodynamics (ISPH) method is presented for the modelling of time-independent non-Newtonian flows. This new method is based on the diffusion-based ISPH methodology by Lind *et al.* 2012 [1] for Newtonian fluids, which has been proven to be stable and accurate, with a virtually noise-free pressure field. The proposed method is validated against internal flows and free-surface flows by comparing with analytical and experimental results respectively. Furthermore, comparisons with previous published results and other CFD techniques were conducted and showed that in addition to the accurate prediction of free-surface flows, the proposed methodology can significantly improve the prediction of the pressure field distribution.

## I. INTRODUCTION

Free-surface non-Newtonian flows are met in a vast variety of applications, both industrial (e.g. lubricants, suspensions, paints, etc.) and environmental (e.g. mud, ice, blood, etc.). Moreover, due to the increased density and viscosity values of these fluids, the pressure and stresses exerted by such flows can be substantial.

Although traditional “weakly compressible” SPH (WCSPH) has proven to be very capable in predicting the kinematic flow patterns of fluids it generally suffers from a noisy pressure field, caused by the explicit density-pressure relationship. This problem is eliminated almost entirely with incompressible SPH (ISPH), first introduced by Cummins and Rudman [2], who used Chorin’s projection method [3] to enforce a divergence-free velocity field. This approach was proven to be substantially better than the WCSPH approach in the prediction of the pressure field, but its applicability was restricted to relatively low Reynolds number due to instabilities occurred by anisotropic particle distribution [4]. Shao and Lo [5] addressed this issue by enforcing the invariance of the density through the pressure-Poisson equation. Although this method improved the particle distribution, it was found to suffer from some noise in the pressure field [4]. A combination of the two aforementioned techniques [6] showed stable and accurate results, with increased computational cost [4], since the pressure Poisson equation now needed to be solved twice.

A promising approach was that of ISPH with shifting first introduced by Xu *et al.* [4], and further improved by Lind *et al.* [1] who used the divergence-free velocity field method,

with the addition of a shifting mechanism based on Fick’s law of diffusion. This approach ensured a uniform particle distribution in the computational domain. This technique has been extensively examined in internal and free-surface Newtonian flows, proving very efficient and accurate in predicting pressure distributions for a wide range of Reynolds numbers and complex geometries [1], [4], [7].

Many attempts have been made in the past to model inelastic non-Newtonian flows with both WCSPH [8]–[11] and ISPH [5], [12], [13]. In general the existing WCSPH and ISPH methods presented well described velocity fields and surface profiles, but rarely showed adequate performance in the estimation of the pressure field. In this work, an approach to non-Newtonian free-surface simulations is introduced, in which ISPH with diffusion-based shifting is expanded to model inelastic non-Newtonian fluids. To validate this incompressible non-Newtonian SPH (INNSPH) method, the following cases are considered: a variety of non-Newtonian internal flows for Bingham and Power-law rheological models, where analytical solutions in the steady state are readily available. A Bingham visco-plastic fluid dam-break case is presented and compared with both experimental [14] and computational results [13]. A more demanding Cross fluid moulding flow problem is also considered and compared with computational results [11]. Traditionally in SPH, pressure results are rarely presented due to the very noisy pressure fields, making it hard to establish the accuracy of the pressure results given by INNSPH. In order to bridge this gap, results of the dam-break problem [14] were compared with a control volume finite element method (CVFEM) [15] available through ANSYS-CFX CFD software. The INNSPH method presented herein, manages to retain the benefits of the SPH methodology in accurately calculating free-surface profiles, in addition to providing a greatly improved estimation of the pressure field.

## II. MATHEMATICAL MODEL

### A. Governing equations

The conservation equations for incompressible flows are as follows:

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

# Buoyancy modelling with incompressible SPH and the unified semi-analytical wall boundary conditions

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**Abstract**—This work aims at modelling buoyancy using a 2D incompressible SPH model (ISPH) where wall boundary conditions are imposed through the unified semi-analytical technique, noted USAW [2]. The model is based on the Boussinesq approximation so that density variations only act through an additional term in the momentum equation. It is combined to a RANS  $k - \epsilon$  turbulence model so as to have a numerical tool able to model industrial or environmental flows. The advantage of working with the USAW boundary conditions, besides their accuracy on complex wall geometries, is that they make it possible to exactly impose arbitrary wall boundary conditions on the temperature. To illustrate this, several configurations of a Poiseuille flow were tested with isothermal walls and/or imposed heat fluxes through the upper wall. In all cases, excellent agreement with the theoretical solution was obtained. We propose several other verifications to the present approach, including a lock-exchange flow, two laminar and one turbulent flow in differentially heated cavities and a turbulent Poiseuille flow. Very good agreement was obtained with mesh-based methods in all cases.

## I. INTRODUCTION

The present work aims at modelling incompressible viscous flows taking active scalars effects into account. Buoyancy plays an important part in many industrial and environmental flows. Modelling its effects through a Lagrangian method presents the advantage of avoiding artificial diffusion, since the convection directly corresponds to the particle displacement. The system of equations to be solved is composed of the incompressible Reynolds-Averaged Navier-Stokes (RANS) equations coupled to a heat equation and to the  $k - \epsilon$  turbulence closure [1]. The buoyancy model was introduced in an incompressible SPH (ISPH) model based on the unified semi-analytical wall boundary conditions (USAW), noted ISPH-USAW [3]. In the equations, the time is noted  $t$ , the gravity  $\mathbf{g}$ , the pressure  $p$ , the density  $\rho$ , the dynamic molecular viscosity  $\mu$ . We define  $\mathbf{v}$ , the Lagrangian velocity and  $\mathbf{u}$ , the Eulerian velocity. Both velocities are equal in our SPH model except for wall particles as we will see in Section II-C. The turbulent kinetic energy is noted  $k$ , and the dissipation rate  $\epsilon$ .  $\mu_T$  is the dynamic eddy viscosity,  $\mu_E = \mu + \mu_T$  is the equivalent dynamic viscosity. We also define  $\nu = \frac{\mu}{\rho}$  and  $\nu_T = \frac{\mu_T}{\rho}$ . The temperature is noted  $T$ , the mean temperature of the flow  $T_0$  and the coefficient of thermal expansion  $\beta$ .  $K_E = K + K_T$

TABLE I  
 VALUES OF THE  $k - \epsilon$  MODEL CONSTANTS [1]

$\kappa$	$C_\mu$	$C_{\epsilon_1}$	$C_{\epsilon_2}$	$\sigma_k$	$\sigma_\epsilon$
0.41	0.09	1.44	1.92	1.0	1.3

is the equivalent thermal diffusivity, with  $K$  the thermal diffusivity and  $K_T = \frac{\nu_T}{Pr_T}$ ,  $Pr_T$  being the turbulent Prandtl number, taken as 0.85. The formalism of heat transfer was chosen, but the reasoning applies to other active scalars like salinity as well. The Boussinesq approximation is used to account for density variations so that  $\rho$  remains constant and the system reads:

$$\left\{ \begin{array}{l} \nabla \cdot \mathbf{v} = 0 \\ \frac{d\mathbf{v}}{dt} = -\frac{1}{\rho} \nabla \tilde{p} + \frac{1}{\rho} \nabla \cdot (\mu_E \nabla \mathbf{u}) + (1 - \beta(T - T_0)) \mathbf{g} \\ \frac{d\mathbf{r}}{dt} = \mathbf{v} \\ \frac{dk}{dt} = \mathbb{P} + \mathbb{G} - \epsilon + \frac{1}{\rho} \nabla \cdot (\mu_k \nabla k) \\ \frac{d\epsilon}{dt} = \frac{\epsilon}{k} (C_{\epsilon_1} \mathbb{P} + C_{\epsilon_3} \mathbb{G} - C_{\epsilon_2} \epsilon) + \frac{1}{\rho} \nabla \cdot (\mu_\epsilon \nabla \epsilon) \\ \frac{dT}{dt} = K_E \nabla^2 T \end{array} \right. \quad (1)$$

The variables  $\mu_k = \mu + \frac{\mu_T}{\sigma_k}$  and  $\mu_\epsilon = \mu + \frac{\mu_T}{\sigma_\epsilon}$  were defined, as well as  $\tilde{p} = p + \frac{2}{3}k$ .  $\sigma_k$ ,  $C_{\epsilon_1}$ ,  $C_{\epsilon_2}$  and  $\sigma_\epsilon$  are constants described in Table I.  $\mathbb{P}$  is the production of turbulent kinetic energy and  $\mathbb{G}$  is a buoyancy production term.  $C_{\epsilon_3}$  is equal to 1 if  $\mathbb{G} \leq 0$  and 0 otherwise. The eddy viscosity  $\nu_T$  is calculated as a function of  $k$  and  $\epsilon$ :

$$\nu_T = C_\mu \frac{k^2}{\epsilon} \quad (2)$$

where  $C_\mu$  is a constant defined in Table I. Note that the eddy viscosity is imposed equal to zero at the walls. In case of a laminar flow,  $\nu_T$  is set to zero and the  $k$  and  $\epsilon$  equations are not solved.

# Modelling buoyancy and thermocapillary convection in molten metals using an incompressible SPH method

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**Abstract**—In laser surface modification of metallic materials characterised by melt displacement, the fluid flow in the molten phase has a crucial effect on the resulting surface structure. In particular, surface tension gradients occurring on the melt surface influence the shape of the molten pool and hence the resolidified material. At first, thermocapillary convection resulting from the temperature dependence of surface tension is considered. In the present article, the test case of a differentially heated cavity filled with liquid metal with an undeformable free surface is concerned. The authors have the impression that the modelling of surface-tension-driven flows is still a less pronounced application of SPH. The prospect is to implement the incompressible SPH algorithm employed here in the thermal model of laser interference patterning to incorporate the molten pool convection and to predict the surface deformation. This capability of SPH will help to understand the physical mechanisms of laser surface modification in detail.

## I. INTRODUCTION

In laser materials processing of metals, incident radiation is absorbed and heats the material to the melting point. Subsequently, the enthalpy of fusion is provided by further absorption of radiation and the molten material is heated. Normally, the supplied intensity of laser irradiation is limited to such an extent that desired material ablation or displacement takes place in the molten phase. Because of the often non-uniform intensity distribution of the laser radiation and its limited extent, the exponential decay of absorbed intensity with depth of penetration and due to heat conduction, temperature gradients occur in the material. In particular, tangential temperature gradients on the molten pool surface cause gradients of surface tension due to its temperature dependence and thus induce thermocapillary convection. For pure metals, surface tension decreases with increasing temperature of the melt. Consequently, thermocapillary convection, or Marangoni convection, in shallow surface layer of the molten pool is directed towards regions of higher surface tension, i.e. towards lower temperature of the melt on the molten bath periphery in pure metals, cf. [1]. The associated displacement of fluid and altered temperature distribution inside the molten pool necessitate the consideration of buoyancy effects as well.

Thermocapillary convection is assumed to be a possible cause of deformation of the molten pool surface. In this regard, Seidgazov [2] proposed that there is a threshold in absorbed laser intensity characterised by a change of the flow structure from vortical flow to shear flow. The present authors believe that this is a reasonable assumption, since they have observed experimentally similar surface deformation in direct laser interference patterning of steel substrates. On the other hand, a different conceivable physical mechanism of laser surface modification is the melt expulsion due to the evaporation-induced recoil pressure at considerably higher absorbed laser intensity. However, surface structures resulting from such a process are irregular and characterised by the occurrence of spatter. The authors intend to employ SPH in the modelling of laser materials processing owing to its unique feature of representing free surface evolution. Such an approach offers the possibility to represent the molten pool deformation occurring in laser materials processing at moderate intensity in the numerical model. Prospective work consists in extending the developed model towards modelling thermocapillary-driven convection with a deformable surface. Such flows were described by Pimputkar and Ostrach [3] and Sen and Davis [4]. The present authors' aim is to implement the incompressible SPH method in the two-phase thermal model of direct laser interference patterning, cf. [5], to account for the molten pool convection and predict the material displacement, i.e. the free surface deformation.

To the best of the present authors' knowledge, there are only few investigations concerning the application of SPH for modelling surface tension driven flows. On the one hand, Adami *et al.* [6] have employed a weakly compressible SPH method for numerical solution of such flow phenomena. However, they have considered flow driven by a gradient of concentration of surface active solute, or surfactant, i.e. solutocapillary convection. The work of Shigeta *et al.* [7] concerns the simulation of thermofluid flow in an arc weld pool including Marangoni convection using SPH. Tong and Browne [8] have modelled heat transfer and fluid flow in the melt pool in laser spot welding considering Marangoni flow

# Space Potential Particles as Free-Surface Boundary Condition in Projection-Based Particle Methods

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**Abstract**—The paper presents a simple and effective scheme as a novel free-surface boundary condition for enhancement of the numerical stability and accuracy in projection-based particle methods, namely, Space Potential Particles, abbreviated as SPP. SPP scheme guarantees accuracy of the volume conservation and physical freedom of motion even for particles around free surface by a particle-void interaction, which is an essential key to keep consistency between physical and mathematical space potential. By performing a set of simple benchmarks including Karman vortex simulations, it is shown that existing models have problems in the volume conservation, specifically about restraint and rectification of unphysical voids, while, SPP scheme shows a good reproduction of this problem with enhancement of accuracy, stability and computational cost.

## I. INTRODUCTION

Projection-based particle methods for viscous incompressible flows, e.g. ISPH (Incompressible SPH) method by Shao and Lo [1] and MPS (Moving Particle Semi-implicit) method by Koshizuka and Oka [2] have been applied to various engineering problems [3,4] owing to their superiority in robustness of tracking free-surface flows. Thanks to the framework based on the Lagrangian tracking, particle methods are free from the non-linear advection term causing numerical diffusion, as a result, are brought a good applicability to complicated violent flows. However, in exchange of this advantage, they require a prudent consideration to the distribution of particles for accuracy and stability in the locally weighted averaging operation. As an approach of this problem, in recent years, the accurate particle methods by introduction of a Taylor consistent correction term [5-10] were proposed with achievement of enhancement of accuracy and stability even with the maldistribution of particles. Nevertheless, considering the volume conservation, the regular distribution of particles is still essential at all times. In particular, this fact comes to be decisive around free surface in the domain due to its deficiency of the particle number density. Needless to say, so is the unphysical free surface, namely unphysical voids. As for a well-known instance of the inconsistent voids, the so-called Karman vortex simulation [11-14] has insufficient trials by particle methods [15-19] due to occurrence of unphysical voids around the centre of vortex, even though the Karman vortex is generally targeted by Grid-based methods for examination of applicability of themselves to the violently complicated flows.

As a rare trial, in the most recent years, Marrone et al. [19] showed a good resolution of this matter by introducing the ghost particles into the interface of a cylinder with good reproduction of vortexes under relative high-order Reynolds number. However, this advancement concentrates on only the flow around the cylinder. Therefore, considering further high-order Reynolds numbers for future work, a careful treatment should be required for unphysical voids which would occur around the centre of strong vortex apart from the cylinder.

For suppression of unphysical voids, it is effective to adopt appropriate models handling the negative pressure [10], which brings particles close to one another so as to diminish directly a dilating cavity between them. However, this concept does not work on voids, but only particles. Therefore, it cannot coordinate voids occurring once, and may result in leaving or expanding their unphysical space. As the second step, the handling of voids should be focused on.

Regarding voids, namely free surface, the projection-based particle methods, e.g. ISPH and MPS frameworks set a free-surface boundary condition with forced zero pressure for a particle whose particle number density is below a threshold. The matrix of the Pressure Poisson Equation (PPE) is solved under this regulation. This process contains two controversial points. First, the free-surface particles are excluded from the Continuity equation without any consideration of the volume conservation for themselves. This problem is clearly shown by overlapped particles around free surface. Second, since the free-surface boundary is treated as a fixed boundary in the matrix of PPE, the sufficient freedom of motion of neighbouring particles for its direction is not guaranteed. That is, existence of the space behind the free-surface particles, where no interaction is defined for the neighbouring particles, is not premised in the mathematical space. Comparing with the physical space, it is clear that this unnoticed factor in the mathematical space brings about a loss of a potential that fluid can be flown into the void space. This fact would be one of the causes of unphysical voids.

Herewith, to resolve the inconsistency in the “Space Potential” between the mathematical and physical space, a new boundary condition for the particle-void interaction as expression of the potential by introducing an additional virtual free-surface boundary particle, namely Space Potential Particles (abbreviated as SPP) is proposed. This scheme sets all



# A Novel Laplacian-Based Surface Tension Model for Particle Methods

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**Abstract**—The paper presents a novel surface tension model for macroscopic particle methods. The proposed surface tension model is based on the Continuum Surface Force (CSF) concept and is characterized by a novel formulation for curvature estimation. The curvature is formulated using direct second order derivatives of color function and is meticulously discretized via a single summation scheme. The new model is referred to as Laplacian-based surface tension model which applies a high-order Laplacian scheme including the approximation of boundary integrals. Comparisons are also made with two commonly applied MPS surface tension models, namely, divergence-gradient based model and the arc fitting one.

## I. INTRODUCTION

Surface tension is caused by the effects of intermolecular forces at the interface. In the bulk of a liquid, the molecules experience equal inter-molecular forces in all directions, while molecules at the interface only feel these forces in one hemisphere and are therefore, pulled inward. This results in a net force towards the bulk in interface regions. In principle, surface tension modelling in the context of particle methods is achieved by either including directly the particle-particle interactions or by considering additional volumetric forces which act directly on the liquid at the interfaces.

The approaches applied for modelling surface tension in macroscopic particle-based methods can be divided into two main categories, namely, the so-called potential approach and the continuum one. The potential approach assumes that microscopic cohesive intermolecular forces can be mimicked by macroscopic inter-particle forces. The major disadvantage of potential approach is related to the fact that the surface tension forces depend on the intensity of particle-particle interactions. These interactions have to be adjusted numerically by varying the macroscopic input parameters depending on the simulation case in order to reproduce desired surface tension forces. Further, with the given parameters, the potential-based surface tension modelling approach is resolution dependent and the modelled surface tension does not converge to a fixed value with resolution refinement [1].

The most common approach for incorporation of surface tension in macroscopic particle-based simulations is based on the Continuum Surface Force (CSF) model introduced by

Brackbill et al. [2]. In this approach, the surface tension is treated as a continuous, three-dimensional effect across the interface, derived directly from the Young-Laplace equation, where the corresponding pressure jump across the interface is applied via a volume force normal to the interface. Morris [3] showed several possible implementations of CSF model in SPH and highlighted one of the most key challenges of this approach, i.e. calculation of interface curvature. This difficulty mainly arises from the fact that interface curvature corresponds to a high order differential operator (Laplacian of a color function) which is usually calculated via a double approximation (or a double summation scheme) comprising of calculations of normalized gradient of a color function and divergence of this estimated normalized gradient.

A set of studies have been carried out on enhancing the particle-based CSF model by providing more accurate schemes for approximation of interface normal and curvature. For instance, Adami et al. [1] proposed a new formulation for the surface curvature by applying a reproducing divergence approximation. Qiang et al. [4] applied a Taylor-series based correction leading to more accurate interface normals and thus curvatures. In most cases, curvature calculation was obtained via a double summation scheme.

An alternative approach for curvature estimation is to formulate it using direct second order derivatives (of color function) and then meticulously discretize it via an accurate single summation scheme. This derivation and discretization have to be performed carefully considering the nature of a continuous and sharp varying color function.

This paper presents a novel and simple surface tension model on the basis of CSF concept and by considering the above mentioned alternative approach. The distinct feature of the proposed model corresponds to accurate estimation of interface curvature via deriving a single summation, Laplacian-based scheme. This derivation has been carried out meticulously by considering the nature of a continuous color function (with bounded values) that varies sharply in a narrow transitional region. The Laplacian-based scheme applies a high-order Laplacian model (analogous to that derived in [5]) and includes approximation of the boundary integrals [6]. This scheme and other considered surface tension models are applied together with an enhanced MPS method [7].

# On the issue of interface spurious fragmentations in multiphase SPH

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**Abstract**—The purpose of the present paper is to investigate the issue of spurious interface fragmentation in Smoothed Particle Hydrodynamics (SPH) approaches for multiphase flows. Although SPH has become an increasingly popular method for free-surface flows, which are addressed as single-phase flows, it has appeared in recent years that current SPH formulations, which have been developed for multiphase flows involving an interface between immiscible phases, can suffer from non-physical particle mixing through the interface. This question is related to spurious fragmentations of interfaces and is an important issue that can hinder specific applications where physical phenomena take place at the interface itself, such as phase change or even changes in two-phase flow patterns. In this paper, the various remedies proposed in the literature are discussed as well as the current assumption that this problem occurs only when there is no surface tension at the interface. It is shown, however, that spurious interface fragmentation is a general problem of current SPH formulations and appears even when surface tension is present. A new proposition for an interface sharpness correction term is proposed and a series of detailed simulations of two and three-dimensional bubble rising in a liquid allow a comprehensive study to be carried out which provides new insights into the relations between the new correction term and central SPH notions such as the kernel smoothing length.

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## I. INTRODUCTION

Due to the Lagrangian nature of the Smoothed Particle Hydrodynamics approach, a strong advantage over Eulerian techniques is that numerical grids are not needed. Consequently, for multiphase flows, the shape of the interface does not have to be reconstructed (contrary to Volume-Of-Fluid, Level-Set or Front-Tracking methods), since it is directly obtained from the set of computational particles.

One of the main advantages of the SPH approach, namely the simulation of interface shapes obtained directly from particle locations, can nevertheless lead to the appearance of a new problem which is a spurious fragmentation of interfaces. This spurious fragmentation is due to an artificial mixing of particles belonging to immiscible phases across the interface, which can then lose its sharpness and becomes locally blurred or slightly fuzzy. As such, this problem is sometimes referred

to as the micro-mixing problem. However, this terminology is misleading since micro-mixing is typically related to a real and physical mixing at microscopic (or molecular) level whereas, here, we are concerned with an artifact happening in the absence of any real molecular mixing. It is thus proposed to refer to this issue as being a spurious fragmentation of interfaces. As it transpires from these explanations, the main reason for the phenomenon of spurious fragmentation is a lack of mechanism assuring immiscibility of phases in the detailed implementations of present SPH formulations. Indeed, in the Eulerian approaches, the precise location of interfaces is given explicitly (at least, locally in any cell) and, therefore, this problem does not occur in these methods. In order to fully benefit from the advantage mentioned above which is provided by SPH simulations, it appears important to address the issue of interface spurious-fragmentations.

A similar behavior in SPH calculations was also reported in [1] and later in [2], but these authors suggested that the problem appears only when surface tension is negligible. To control interface sharpness and prevent spurious interface fragmentations, some authors have proposed various forms of small repulsive forces acting on particles located close to the interface, cf. [1], [2], [3]. One recent approach, which differs qualitatively from previous ones, was proposed in [4], where the authors suggested to smooth the density and viscosity of fluids in order to avoid sharp gradients of fields close to the interface. It is thus seen that this issue is receiving more and more attention.

In the present work, we focus mainly on this issue of spurious fragmentation of interfaces in SPH formulations. Remedies which have been put forward in the literature will be first discussed and a new variant of the sharpness correction procedure, based on the multiphase SPH formulation by Hu and Adams [5] is proposed. Detailed analysis of two- and three-dimensional simulations of a bubble rising in a liquid confirms that such correction terms are required in present SPH computations. A careful and comprehensive study of the influence of the new proposal for the sharpness correction term brings out some insights into the relation between intrinsic parameters. Furthermore, the influence of key computational parameters of a SPH formulation, such as the smoothing length

# Numerical simulation of jet fragmentation in multi-fluid medium using Smoothed Particle Hydrodynamics

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**Abstract**—The Rayleigh-Plateau instability governs the fragmentation of a low Weber number hydrodynamic jet in a multi-fluid medium. Therefore, the SPH simulation of a hydrodynamic jet at high density ratio requires a multi-fluid model and a surface tension model which accurately handle the necking behaviour where the jet eventually breaks into droplets.

In this paper, we apply the surface tension model of [1] motivated by continuum surface force (CSF). The surface tension model is validated against the Young-Laplace pressure for droplets of small diameters  $\mathcal{O}(10^{-3})$ . In addition, the Neumann boundary condition near the interface to allow for the discontinuous pressure jump due to surface tension. The combination of surface tension model and the multi-fluid SPH formulation successfully demonstrates the break-up (or fragmentation) of a hydrodynamic jet, where the density ratio of the liquid jet and ambient gas is 1000.

Three validation cases are presented to evaluate the combination of these models: (i) the square box test, (ii) the static droplet pressure comparison between SPH and the Young Laplace pressure, and (iii) the oscillation of a droplet in multi-phase medium.

The jet break up is simulated using the multi-fluid SPH, with surface tension. The break-up time is found to be dependent on the amplitude of the initial perturbation, the density ratio and the viscosity. The linear relation between break-up time and initial perturbation amplitude has a slope of -0.12 and an intercept of 0.328. Whereas the linear dependence between break-up time and artificial viscosity parameter has a slope of 0.04 and intercept of 0.05.

## I. INTRODUCTION

A jet is a stream of matter organised into a collimated shape. Jets span a large variety of length scales and are encountered in many scientific and technological applications such as the design of propulsion systems, diesel engines, ink-jet printers, and nuclear fusion experiments. Rayleigh [11] and Plateau [10] conducted a linear stability analysis to study the break-up of a jet, therefore, the Rayleigh-Plateau instability (RPI) is named after them. Their work was later extended by Lafrance [7], who conducted a third order perturbation analysis of an inviscid liquid jet. The author found the interaction among non-linear terms is responsible for the generation of satellite droplets.

With the advances in computer technologies, some research groups have conducted numerical simulations of the RPI. Mead-Hunter et al. [8] simulated the RPI occurring around an optical fiber with the combination of finite volume method

(FVM) and volume-of-fluid (VOF). Choi et al. [3] simulated the capillary instability of nano-scale surface tension driven flow of a Lennard-Jones fluid by means of molecular dynamics (MD). The authors reported good agreement with classical theories and claimed that the thermal fluctuations are responsible for the break-up of nano-scale jets.

The past decade has also witnessed the growth of applying particle methods in jet simulations. Shibata et al. [13] simulated the jet break-up using a Moving Particle Semi-implicit Method (MPS). Their study focussed on the effects of the Weber number and Froude number. The authors reported the breakup length deviated from the experimental data by 70%-80%, whereas the relative error of 25% was reported when the influence due to gravity was neglected. Similarly, Takashima et al. [15] simulated the break-up process by means of Incompressible SPH (ISPH) and reported good qualitative agreement with the experimental results, except for the pinch-off length. Recently, Sirotkin and Yoh [14] introduced the corrected smoothed particle hydrodynamics (CSPH) method for simulating surface tension driven flow. Their numerical scheme is based on the combined use of continuity equation approach (for density evaluation) and the surface tension model of Morris [9]. They simulated the two-dimensional jet break-up without taken into account the ambient fluid and found acceptable agreement for the critical Weber number which governs the transition from the jetting to dripping.

This work presents the results of a three-dimensional hydrodynamic break-up modelled with weakly compressible SPH (WCSPH). While variants of SPH have been applied for jet simulation [13, 14, 15], to the authors' best knowledge, a three-dimensional break-up of a hydrodynamic jet has never been attempted with WCSPH. More importantly, we consider the break-up of a hydrodynamic jet submerged in an ambient fluid for the density ratio up to 1000. The combination of high density ratio and small jet diameter therefore challenges the capability of the state of the art SPH models.

The rest of this paper is organised as follows: section II describes the numerical methods used in this work. A series of simulations are conducted in section III to validate the SPH scheme. The SPH results of the Rayleigh-Plateau instability are presented in section V. Finally, we summarise our findings in Section VI.

# Implementation of surface tension in polymer flow during Reactive Rotational Molding

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**Abstract**— The Reactive Rotational Molding (RRM) is a molding process where the polymer synthesis and shaping of piece is carried simultaneously. The main drawback of RRM is poor control of the process due to the high number of influent parameters. In this condition, the optimization of the process is quite complex. Homogeneous quality in technical parts requires the mastery of the process by controlling on line the main physical parameters. During RRM, it is very important to predict the fluid flow in order to be able to obtain the piece with homogeneous shape and with high quality. For this study, Smoothed Particles Hydrodynamics (SPH) have been applied to simulate the polymer flow during this process. Indeed, SPH method is a suited method to simulate the fluid flow with free surface. To implement tension surface force, the interface between polymer and air is tracked dynamically by seeking the particles constituting this border. First, the boundary particles are detected by free-surface detection algorithm developed by Brecasco, Terissa and NAA[1,2]. Then, two methods were used to reconstruct the interface, the Lagrangian interpolation and fitting circle in two dimensions SPH solver. Finally, the results obtained by both methods, have been compared together. The simulation is validated by comparing the numerical results with experimental measurements of dam break problems. Then, 2D simulations were performed for flow polymer during RRM.

## I. INTRODUCTION

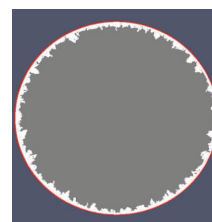
Rotational molding is a four-stage, high-temperature (150°C-300°C), low-pressure, plastic molding process that uses heat and bi-axial rotation to produce hollow, one-piece parts [3-4].

Rotational molding is an economically and environmentally viable method for manufacturing of polymers. The molds of this process are less expensive because it's not necessary to make them with high performance materials. In absence of pressure, there is not residual stress in final parts. In this manufactory method, the quantities of wasted materials are low. However, this process takes long times, about 20-40 minutes; so this technique is generally used for small series of industrial parts. The limited number of polymers only thermoplastics that can be used for rotational molding is also considered as another disadvantage of this process. The various inconvenient of conventional rotomolding have favored the emergence of Reactive Rotational Molding (RRM) where the polymer synthesis and piece shaping are carried simultaneously which allows to reduce the cycle time and expand the range of materials such as thermoset [4]. Modeling of this process is a

challenge because a multiple parameters involved during this process like the rate of chemical reactions, viscosity variations during polymerization and fluid flow during crosslinking. These phenomena are complex and require detailed study to modeling the process.

However, few research works focused on the reactive process unlike conventional rotational molding. The flow during the reactive process, on a cylinder in uniaxial rotation was described for the first time by Throne and Jhonson [5-6], they defined four ideal hydrodynamics regimes occurring during the process.

Finite element calculation based on mesh methods, such as Finite volume method, has been applied to simulate flow polymer during the process, but the calculation wasn't stable and the free surface misrepresented [7]. This is mainly due to the large difference in viscosity and density of the two phases (air-polymer). To overcome this difficulty Mounif[8] and Riviere[9] adopted meshless method called Smoothed Particles Hydrodynamic (SPH) which is best suited to simulate the fluid flow with free surface [10] such as appears in RRM. Riviere's work permitted to enhance the initial solver developed by Mounif by the implementation of rheokinetic model and a new kind of boundary condition to model the adhesion of the reactive fluid on the mold surface. Unfortunately, we observed in the Riviere's solver as it works can generate roughness or particle agglomerates on the internal surface (Fig.1) because the material adhered to this surface can't be deformed. This phenomenon affects the flow of material and its adhesion process that can be slowed and even stopped. It will also consider this problem for example by integrating new model or criterion then seeing if taking into account the viscoelasticity of the material and / or surface tension, this phenomenon can be reduced. In this study, the surface tension force will be integrated in SPH solver in order to simulate the polymer flow during reactive rotational molding process.



**Fig.1:** formation of particle agglomerates on the internal surface of mold. The mold is shown in red, the adhered material in white.

# Exact computation of SPH wall renormalising integrals in 3-D

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**Abstract**—New approaches in modelling wall effects in SPH are based on wall renormalising integrals. In one of the most recent approaches (Ferrand *et al.* [1]), the discrete differential operators are modified using boundary terms  $\gamma_a$  and  $\nabla\gamma_{as}$  that are used to discretise the walls. In the present work, we propose a new exact method to compute analytically these quantities in 3-D for the 5th order Wendland kernel. The idea consists of two steps: 1) following Feldman and Bonet's method [2], Gauss's theorem is used to write  $\gamma_a$  as the sum of boundary integrals like  $\nabla\gamma_{as}$ . These boundary terms are integrals over triangles (sometimes truncated by a sphere); 2) using again Gauss's theorem, the boundary integrals are transformed into integrals over edges  $e$  (straight lines), which can be computed exactly. Comparisons against the analytical value of  $\gamma_a$  in special cases like a right-angle edge provide satisfactory results. Although rather time consuming, this algorithm makes it possible to compute boundary terms exactly in 3-D and provides a better prediction of wall pressure. The overall computation time is only increased slightly due to an increased time step.

## I. INTRODUCTION

Recent publications on SPH for fluids use a new method to treat wall boundary conditions, based on boundary terms. In Ferrand *et al.* [1] for example, the discrete gradient operator reads

$$\mathbf{G}_a \{A_b\} \doteq \frac{\rho_a}{\gamma_a} \sum_b m_b \left( \frac{A_a}{\rho_a^2} + \frac{A_b}{\rho_b^2} \right) \nabla w_{ab} \quad (1)$$

$$-\frac{\rho_a}{\gamma_a} \sum_b \rho_s \left( \frac{A_a}{\rho_a^2} + \frac{A_s}{\rho_s^2} \right) \nabla \gamma_{as} \approx (\nabla A)_a$$

where  $a$  and  $b$  stand for the particles while  $s$  denotes wall boundary elements called 'segments'. The latter are line segments in 2-D and polygons (most of time triangles) in 3-D. This approach, which can easily be extended to other operators like the divergence and Laplacian, has proved being efficient to model wall effects under all circumstances. The main difficulty is to estimate the boundary terms, which are defined as

$$\gamma_a \doteq \int_{\Omega} w(|\mathbf{r} - \mathbf{r}_a|) d^n \mathbf{r} \quad (2)$$

$$\nabla \gamma_{as} \doteq \mathbf{n}_s \int_s w(|\mathbf{r} - \mathbf{r}_a|) d^{n-1} \mathbf{r}$$

where  $w$  is the kernel and  $n$  the space dimension.

Ferrand *et al.* [1] have explained how to compute  $\nabla\gamma_{as}$  exactly in 2-D as a function of the position of particle  $a$  and the position, orientation and length of the wall segment  $s$ . These authors used a time governing equation to deduce  $\gamma_a$ , needing an additional stability condition for the time step. Later on, Leroy *et al.* [3] showed how to compute analytically  $\gamma_a$  in 2-D without any governing equation, starting from an idea of Feldman and Bonet [2]. Finally, Mayrhofer *et al.* [4] proposed a relatively complex algorithm to compute  $\nabla\gamma_{as}$  exactly in 3-D. To our knowledge, no algorithm has been published so far to compute  $\gamma_a$  exactly in 3-D. Our purpose is to provide a new algorithm to compute  $\gamma_a$  and  $\nabla\gamma_{as}$  analytically in 3-D, on the basis of the Wendland kernel of order 5:

$$w(q) = \frac{\alpha_{W,n}}{h^n} \left(1 - \frac{q}{2}\right)^4 (1 + 2q) \quad q \leq q_{\max} = 2 \quad (3)$$

where  $q = r_{ab}/h$ ,  $h$  is the smoothing length and the normalising constant is  $\alpha_{W,3} = 21/16\pi$  ( $\alpha_{W,2} = 7/4\pi$  in 2-D).

In comparison to the algorithms where  $\gamma$  is computed from a time governing equation, the present approach will allow increasing the time step, as we will see.

## II. WRITING $\gamma_a$ AS A BOUNDARY INTEGRAL

Here we show how Feldman and Bonet's approach [2] can be extended to 3-D to write  $\gamma_a$  as a boundary integral.

### A. Feldman and Bonet's approach

We start by summarising Feldman and Bonet's idea. It consists of writing  $w(q) = \text{div} \mathbf{W}(q)$ , which makes it possible to use Gauss's theorem:

$$\gamma(\mathbf{r}) = \int_{\Omega} w(|\mathbf{r} - \mathbf{r}'|) d^n \mathbf{r}' \quad (4)$$

$$= - \int_{\partial\Omega} \mathbf{W}(|\mathbf{r} - \mathbf{r}'|) \cdot \mathbf{n}(\mathbf{r}') d^{n-1} \mathbf{r}'$$

where  $\mathbf{n}$  is the inward unit boundary vector. Since  $w$  is a radial function,  $\mathbf{W}$  must have the same property, *i.e.*  $\mathbf{W}(q) = -\varphi(q) \tilde{\mathbf{r}}$  with  $\tilde{\mathbf{r}} = \mathbf{r} - \mathbf{r}'$ . Thus:

$$\gamma(\mathbf{r}) = \int_{\partial\Omega} \varphi(q) \tilde{\mathbf{r}} \cdot \mathbf{n}(\tilde{\mathbf{r}}) d^{n-1} \tilde{\mathbf{r}} \quad (5)$$

# Local Uniform STencil (LUST) boundary conditions for 3-D irregular boundaries in DualSPHysics

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**Abstract**—In this paper, a novel 3-D wall boundary treatment for SPH is developed. Boundary surfaces are discretized into sets of triangular planes. Boundary particles are then obtained by translating a full uniform stencil according to the fluid particle position and applying an efficient ray casting algorithm to select particles inside the fluid domain. The method ensures that a complex geometry can be readily discretized while guaranteeing approximate zeroth and first order consistency. No special treatment for corners and low computational cost make the method ideal for GPU parallelization. The proposed algorithm is coded in the open-source software DualSPHysics. Static and dynamic test cases are used to validate the wall boundary model. Significant improvements over the pre-existing wall boundary condition of DualSPHysics are demonstrated.

## I. INTRODUCTION

Imposing boundary conditions (BCs) in SPH is still an open problem due to the Lagrangian nature of SPH and the kernel based interpolation. Therefore the extension of many boundary conditions to 3-D problems can be cumbersome. A widely used approach, proposed by Monaghan [1-2], is the repulsive force method where the wall is described by particles which exert a repulsive short-range force similar to a Leonard-Jones potential force on fluid particles. With this approach 2-D and 3-D irregular geometries can be easily discretized, but the kernel truncation near the wall can introduce non-negligible inaccuracies.

Another widely used method to describe boundaries in SPH [3-4] is the mirror or ghost particles as introduced by Randles and Libersky [5]. However, extending the method to 3-D is challenging for irregular geometries. Kulasegaram et al. [6] proposed a variant of this method which introduces an additional term in the momentum equation in order to mimic the effect of the wall. This technique eventually uses an empirical function originating from variational principles to approximate the force, the concept was further developed in [7-10]. These methods have the advantage of restoring zero-consistency in the SPH interpolation but the discretization of complex 3-D geometries and/or multiphase flows is not straightforward [11].

Ferrari et al. [12] proposed a local point symmetry method which is able to discretize arbitrarily complex geometries without introducing empirical forces. Recently the method was

further enhanced and applied to shallow water equations (SWE) [13] and Navier Stokes equations [14] in 2-D.

In this work the latter method is extended to 3-D arbitrarily complex geometries. The wall boundaries are described by triangles to maximize the efficiency, also for GPU parallelization. Approximate zeroth and first order consistency are ensured by using a fully uniform fictitious particle stencil.

The proposed wall boundary condition is implemented in the open-source code DualSPHysics [15]. The dynamic boundary condition (DBC) [3] currently implemented in DualSPHysics is suitable to reproduce complex geometries but suffer from drawbacks such as over-dissipation and spurious pressure oscillation. Therefore, a new accurate wall boundary is needed.

The paper is organized as follows; Section II briefly recalls the governing equations, the novel local uniform stencil wall boundary condition (LUST) method is presented in Section III, Section IV highlights the numerical implementation in GPUs and finally in Section IV the numerical scheme is tested against reference solutions.

## II. GOVERNING EQUATIONS

This Section presents the governing equations in SPH form. Throughout this paper, subscripts  $i$  and  $j$  denote the interpolated particle and its neighbours respectively. The density evolution and momentum of the particles follow the Navier-Stokes equations [16]

$$\left\{ \begin{array}{l} \frac{d\rho_i}{dt} = \sum_j^N m_j \mathbf{u}_{ij} \cdot \nabla_i W_{ij} + D_i \\ \frac{d\mathbf{u}_i}{dt} = \sum_j^N m_j \left( \frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_i^2} + \Pi_{ij} \right) \nabla_i W_{ij} + \mathbf{g}_i, \\ \frac{d\mathbf{x}_i}{dt} = \mathbf{u}_i \end{array} \right. \quad (1)$$

where  $\mathbf{x}_i$  is the position,  $\mathbf{u}_i$  is the velocity,  $\rho$  is the density,  $P$  is the pressure,  $m$  is the mass and  $\mathbf{g}_i$  is the gravity acceleration. In this paper, the Wendland kernel [17] has been used as a smoothing function but numerical tests have shown similar

# Explicit Strategies for Consistent Kernel Approximations

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**Abstract**—The paper reports investigations on explicit strategies for consistent kernel-based approximations of functions and derivatives to be used in SPH. The study is motivated by the challenges of truncated and irregular (unsymmetrical) particle samplings in conjunction with non-collocative standard kernel based approximations. Examples of such problems refer to the imposition of boundary conditions or predicted spurious gradients of homogeneous fields. Therefore a transition to a more cardinal basis in the vicinity of boundaries as well as an adjustment to sampling irregularities might be desirable. Attention is devoted to consistency properties up to the order of 2 derived from a 1D analysis. Emphasis is given to explicit corrections in discrete space rather than appropriate analytical formulations in continuous space. The strategy here presented is compared with former (implicit) approaches suggested by Chen and Beraun [1] as well as Liu and Liu [2]. Deficits of explicit second-order accurate approaches and routes towards multiple dimensions are discussed. Results indicate benefits of consistent approaches as regards the formulation of boundary conditions with only one row of particles.

## I. INTRODUCTION

Consistent kernel approximations represent a challenge in Smoothed Particle Hydrodynamics. The consistency returned by isotropic bell-shaped kernels is rigidly linked to the location of particles inside the support domain. They are second-order accurate for a "lattice" of regularly spaced particles if the particles are located far from the boundaries of the wetted domain. In this case, the symmetry and compact support properties are also valid in discrete space. Particularly, the inherent symmetry of the kernel function  $W_{ij}$  together with a symmetric spacing of neighbours  $x_j$  around  $x_i$  yields  $\sum_j W'_{ij} \sim \sum_j W_{ij}(x_i - x_j) = 0$  and is an important feature of the predictive performance and the attainable order of accuracy. On the contrary, the kernel-based approximation suffers from severe consistency and accuracy problems when irregular sampling occurs or the support regime is truncated close to the centre, which e.g. is a frequently met issue along boundaries.

A number of techniques to improve the kernel function or its derivatives have been published. They all aim at achieving an enhanced level of consistency and predictive accuracy. The improvements are related to a sequence of conditions for sums of the central moments of the kernel function and its derivatives which must either vanish or achieve unity. The

most popular variant is the Shepard normalisation of the kernel function itself [3], which provides zero-order consistent approximations of functions but not of gradients. More advanced examples of formerly published strategies are the reproducing kernel method [4] or the moving least-square approach of Dilts [5], [6], which reveal some similarities [7], [8] and the two series expansion based suggestions of Chen & Beraun [1] and Liu & Liu [2]. Unfortunately, all these approaches refer to implicit techniques and involve the solution of equations systems for each particle at each instant of time. The size of the equation system scales with the consistency order and the dimensionality of the problem.

The goal of the present study is to investigate means for an explicit corrective procedure to improve the consistency of the smoothing function. Due to their importance in kernel-based approximations of transport equations, emphasis is given to improvements of gradient approximations. Different from many other strategies the present techniques is derived in discrete space, which naturally supports irregular particle locations and facilitates apparently simple explicit corrections at moderate computational surplus of a few additional neighbour loops.

The remainder of the paper is structured as follows: The employed SPH model and the respective background of the consistency requirements are briefly repeated in the second section. The third section is devoted to explicit corrections up to the order of two in 1D. The fourth section deals with two different applications, i.e. a lid-driven cavity flow at  $Re=400$  &  $Re=1000$  and a simplified 1D channel flow. Final conclusions are drawn in the fifth section.

## II. MATHEMATICAL MODEL

This section briefly outlines the governing equations and their SPH-based approximation of fluid dynamic problems in addition to a short overview on consistency constraints. The subscript  $i$  indicates the focal particle, while  $j$  refers to neighboring particles found inside the kernel support. Vectorial and tensorial quantities are indicated by bold symbols. Cartesian coordinates of tensorial quantities are distinguished using greek superscripts. Spatial derivatives in direction  $\alpha$  are indicated by  $(...)^{\alpha}$ .

# Open Boundary Conditions Using the Mirror Ghost Particle Approach in OpenFOAM SPH

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**Abstract**—A new algorithm for inlet/outlet boundary conditions in the context of Smoothed Particle Hydrodynamics (SPH) is proposed in this paper. The algorithm manages the insertion and extraction of particle mass and particles. At the inlet, the particles are accumulating mass according to prescribed mass fluxes, whereas, at the outlet, the relative movement between the particles and the outlet is determining the removal of particle mass. A mirror ghost particle approach is used to impose the boundary conditions and to maintain an almost homogeneous particle distribution across the open boundaries, while avoiding the explicit control of the temporal evolution of the boundary particles.

The algorithm is validated with a 2D Poiseuille flow test case at low Reynolds number. Good agreement with the analytical solution is found for an increased ratio of smoothing length to initial particle spacing. However, using low smoothing lengths, the density of particles close to the boundary exhibits instabilities, which prohibit a steady state solution. An analysis of the instabilities, caused by the continuous redistribution of mass within the kernel of those particles, is presented in terms of a 1D numerical experiment. A suitable correction approach is subject for future investigation.

## I. INTRODUCTION

The primary atomization of liquid fuels including water/fuel emulsions plays a crucial role in the control of emissions for power generation gas turbine engines operating in fuel oil. Furthermore, it is one of the most challenging physical models in the chain of physical phenomena involved in fuel oil combustion.

Due to its computational efficiency, Euler-Lagrangian algorithms are often used for simulating liquid sprays in combustors [1]. This method uses Lagrangian parcels representing a certain bunch of droplets, which are interacting through appropriate source terms with the gas phase being represented by an Eulerian approach. The trade-off for the computational efficiency is the extremely simplified description of the phase interactions, which is most often based on semi-empirical correlations. Contrarily, completely grid based approaches derived from the Finite Volume (FV) method, e.g. Volume of Fluid (VOF), resolve the phase interfaces directly [2]. These advanced approaches rely on computationally costly interface reconstruction techniques. Therefore, in case of the breakup of water/fuel emulsion jets the large number of phase interfaces may become cumbersome for those methods.

To overcome those shortcomings, the Institute for Thermal Turbomachinery (ITS) started to develop a Smoothed Particle

Hydrodynamics (SPH) code [3]. This method has the inherent advantage of the natural advection of phase interfaces, which simplifies the numerical handling of the phase interactions. Since SPH has indeed certain drawbacks compared to grid based methods (e.g. treatment of boundary conditions, strong time step restrictions, large interaction stencil) [4], a coupling of both methods will provide advantages towards the realization of simulations of the technical liquid jet breakup. In this context, the principle idea is to utilize SPH in regions, where strong phase interactions take place, i.e. the jet breakup region. On the other hand, it is desirable to benefit from the high accuracy and efficiency of the FV method in single phase regions and regions, where the phase interactions may be captured by semi-empirical correlations with sufficiently high accuracy, i.e. upstream and downstream of the primary atomization zone. Thus, downstream of the primary atomization zone an Euler-Lagrangian solver needs to be applied to manage the droplet-gas interactions. Since the most convenient way of coupling two numerical methods is to use the same code environment, SPH was implemented into the open source CFD toolbox OpenFOAM [5] during this work and is intended to be coupled with the FV method in the future.

An interesting approach for coupling SPH with a different numerical method (incl. the FV method) was recently presented [6]. The domains of the coupled solvers use overlapping interfaces, in which the particles are behaving according to the solution of the external solver. However, due to the temporal evolution of those particles, a computationally expensive particle seeding algorithm is required in order to ensure a sufficiently homogeneous distribution of particles at the interface.

At the interface between a SPH domain and a FV grid, particles may leave and new particles may enter the SPH domain. Therefore, this situation is strongly related to inlet/outlet boundaries in SPH, which has only been addressed in a few publications, e.g. [7], [8] and [9]. Generally, buffer zones are connected to the inflow and outflow boundaries. Particles, which are located inside the inflow buffer, behave according to a prescribed velocity profile. As soon as a buffer particle is moving from the buffer zone into the internal domain, a new buffer particle has to be inserted at the entry of the buffer zone. This approach shows some similarity to the particle seeding mentioned above, even though, in a very simplified



# Multi-GPU, multi-node SPH implementation with arbitrary domain decomposition

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**Abstract**—We present a restructured version of GPUSPH [4], [8], [11], a CUDA-based implementation of SPH. The new version is extended to allow execution on multiple GPUs on one or more host nodes, making it possible to concurrently exploit hundreds of devices across a network, allowing the simulation on larger domains and at higher resolutions. Partitioning of the computational domain is not limited anymore to parallel planes and can follow arbitrary, user-defined shapes at the resolution of individual cells, where the cell is defined by the auxiliary grid used for fast neighbor search. This allows optimal partitioning even in the case of complex domains, such as rivers with U-turns. The version we present also includes many additional features that have been developed on GPUSPH. Particularly important are: the uniform precision work by Hérault *et al.* [13], which is essential for numerical robustness in the case of very large ratios between the domain size and particle resolution; a compact neighbor list, which allows larger subdomains to be loaded on each device; the semi-analytical boundary conditions by Ferrand *et al.* [9], [12], and support for floating objects [14]. All of these features are seamlessly supported in single-GPU, multi-GPU and multi-node modes.

## I. INTRODUCTION

From a computational perspective, one of the most important benefits of the weakly-compressible Smoothed Particle Hydrodynamics (SPH) numerical method is its embarrassingly parallel nature. This has led to a number of implementations of SPH for high-performance parallel computing platforms, most recently focusing largely on Graphic Processing Units (GPUs) [4], [5] and similar architectures, which have shown to be very efficient alternatives to traditional CPU clusters both in terms of performance/price and in terms of performance/power consumption ratios.

GPUs hold tens of compute units with hundreds of processing elements which operate in parallel to concurrently execute a large number of instances of *computing kernels*, the equivalent of standard CPU functions, in a shared-memory model (all processing elements can access the same global memory), allowing a well-tuned GPU program to easily perform  $100\times$  faster than equivalent serial CPU implementations.

Limitations in GPU usage are largely determined by memory occupation, since even the most expensive, compute-dedicated GPUs are currently limited to 6GB of RAM for a single device, almost an order of magnitude less than the amount of memory that can be found on a high-end workstation. To circumvent this limitation, and to further reduce runtime, a second level of parallelism needs to be introduced, by using multiple GPUs connected to the same host CPU.

Multi-GPU usage in SPH has been shown in [8], [10], [11], and is based on the principle of domain decomposition, where each device is assigned either a fraction of the total amount of particles in the simulation, or a section of the computational domain. Compared to single-GPU programming, using multiple GPUs introduces a layer of complexity due to the distributed memory (each device only has access to a fraction of the entire particle system) and the need to exchange data between different devices.

In this paper we present an enhanced version of GPUSPH, that introduces an additional layer of parallelism by allowing the distribution of the computation across multiple GPUs connected to multiple host machines. To achieve this, the multi-GPU version of GPUSPH [8], [11] has been restructured, removing restrictions in the domain decomposition, refactoring data transfers to allow transparent network usage, and including a number of enhancements such as homogeneous precision (see Hérault *et al.* elsewhere in these proceedings) which are essential to avoid numerical issues in the large-scale high-resolution simulations which are made possible by the new opportunity to distribute computations across hundreds of devices.

We will first present an overview of the general and technical features of GPUSPH for single devices (section II), which will provide a basis to introduce the changes necessary to support multiple devices on one or multiple host machines, discussed in section III with the implementation details and technical challenges. Results are presented and discussed in section IV-B, leading to the conclusions in section V.

# Achieving the best accuracy in an SPH implementation

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**Abstract**—Most SPH implementations use a naive approach which is a literal translation of the mathematical formulas for SPH into computer code. This does not take into account the fact that computer floating point arithmetic does not obey many of the common properties of real numbers arithmetics. For example, addition and multiplication are not associative in floating point, and the accuracy of any operation is proportional to the value of the least significant digit of the involved numbers which are larger in magnitude. We propose a new approach which ensures that all SPH computations are done at the maximum possible accuracy, uniformly across the entire domain. The main key point of the approach we propose is to never use global, absolute positions, but instead use positions local to the cell grid used for neighbor search. Additional benefits can be gained by using a similar approach for density, by the use of Horner’s scheme to compute the equation of state, and finally by using Kahan summation for integration.

## I. INTRODUCTION

In 1984 the IEEE put an end to the chaos in the representation and treatment of floating-point values throughout computer architectures, finalizing the standard (IEEE-754) that has been adopted by all manufacturers since.

The basis of the standard is a common structure for the representation of floating-point values, with different levels of precisions achieved by similarly-coded formats whose only difference is the width of the type in bits. A floating-point value is represented by a sign bit  $s$ , an integer exponent  $p$  (stored in biased form), and a (binary) mantissa  $c$ . The represented value is thus  $(-1)^s \cdot c \cdot 2^p$ . The mantissa itself represents a fixed-point value between 1 (inclusive) and 2, but the leading 1 is implicit, to gain 1 bit of accuracy in the representation.

The standard also includes provisions for special values, such as (signed) infinity, denormal numbers (numbers smaller than the smallest representable value in normal form, characterized by having an exponent of 0 and not assuming an implicit 1 in the mantissa) and even not-a-number (NaN) values, typically obtained as the result of indefinite operations such as 0/0.

The most common formats supported in modern hardware are the single-precision “binary32” format (fp32), typically

represented in the C family of programming languages by the `float` type, and the double-precision “binary64” format (fp64), typically represented in the C family as the `double` type. The bit widths of the exponent and mantissa for these types are shown in table I.

An interesting side-effect of the representation of floating-point values by the IEEE-754 is that the density of the representable real numbers is not uniform throughout the real line: since the mantissa has a fixed width, the distance between two consecutive representable number is given by the actual numerical value of the least significant bit, which is essentially controlled by the value of the exponent: in a format with  $M$  bits of mantissa, the least significant bit has value  $2^{(p-M)}$ , where  $p$  is the exponent. This value is known as “Unit of Least Precision” (ULP). For example, in single precision with an exponent of 3 this value is  $2^{(3-23)} = 2^{-20} = 9.53 \cdot 10^{-7}$ . The ULP for exponent 0 is known as machine epsilon and in this paper will be written as  $\epsilon_m$ . Values for  $\epsilon_m$  and the largest and smallest (normal) representable numbers are shown in table I.

A direct consequence of the representation is that representable floating-point values are “more dense” towards 0 and get sparser as the magnitude (absolute value) of the values grow. In fact, beyond a certain point not even all integers are representable: in single-precision, the limit is  $2^{24}$ , for which the next representable value is  $2^{24}+2$  (meaning that 16777217, which is not representable, will be converted to 16777216.0 under the standard round-to-nearest-even rounding mode), up to the next power of two, where numbers are spaced by 4 units, and so on.

The decreasing density of representable numbers has important consequences in applications, and it can lead to surprising results, or even introduce subtle bugs in operational code. The effect is seen when adding (or subtracting) numbers whose ratio is lower than machine precision: adding two numbers  $L$  and  $s$  with  $|s/L| < \epsilon_m$  results in  $L$  (i.e. with floating point arithmetics  $L + s = L$ ). More in general, addition and multiplication with IEEE-754 numbers are not associative [ $(a + b) + c$  results in a value which is generally different

# Efficient implementation of double precision in GPU computing to simulate realistic cases with high resolution

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**Abstract**—Single precision has been used in past SPH simulations and it has been shown to be sufficiently accurate for most of the applications considered so far. However, the latest developments for hardware acceleration using GPU computing have led to an important increase in the size of the simulations and new cases have appeared where single precision is insufficient and new solutions must be investigated. Thus, problems originating from the lack of precision can appear in simulations of very large domains which also require a very high resolution. Typically, problems arise when domains of hundreds of meters are studied with resolutions of centimetres or millimetres. The aim of this work is to address when and why these problems of precision appear and which are the best solutions in terms of efficiency for GPU executions.

## I. INTRODUCTION

High performance computing provided us with the tools needed to perform huge simulations at a reasonable computational runtime. Therefore, new simulations for real engineering problems can be computed with SPH models. The parallel computing power of Graphics Processing Units (GPUs) has led to an important increase in the size of the simulations but problems of precision can appear when simulating large domains with a high resolution.

The goal of this research is to address the problem of the lack of precision and to develop the best solutions increasing the precision but keeping the current efficiency of the GPU codes. The results shown in this work are obtained with the DualSPHysics code ([www.dual.sphysics.org](http://www.dual.sphysics.org)). DualSPHysics [1] is based on the SPH formulation implemented in SPHysics ([2,3]) and has been developed to apply the SPH technique to real engineering problems. The software can be run both on CPUs and GPUs. Details on the implementation of DualSPHysics can be found in [4,5,6]. The model has been successfully applied to the study of some engineering problems such as the computation of forces exerted by large waves on the urban furniture [7] or the study of the run-up in an armour block breakwater [8]. Single precision was used in those applications being shown to be sufficiently accurate.

The GPU implementation of double precision allows simulating real problems where single precision was not enough. This is especially well suited for problems where very different spatial scales are involved. An application case involving surface runoff will be used to exemplify the approach.

## II. THE PROBLEM OF PRECISION

The problems of precision mainly appear when the domain is huge in comparison to the distance of interaction between particles. In Fig. 1, a testbed is presented where the length of the domain ( $L=18\text{m}$ ) is much higher than the initial depth of the fluid ( $D=0.18\text{m}$ ) and huge comparing with inter-particle distance ( $dp=0.01\text{m}$ ). The difference between the maximum and minimum spatial scale is bigger than three orders of magnitude in this case.

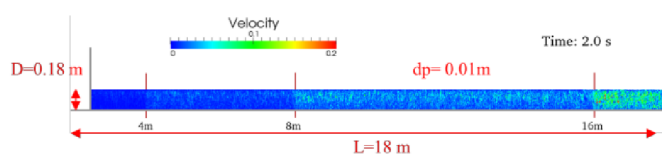


Figure 1. Testbed to study problems of precision.

The origin of the problem comes from the use of single precision for the variables to compute and store the position of the particles. The format of real data in single precision has a size of 32 bits; 1 bit for the sign, 8 bits for the exponent and the remaining 23 bits for the mantissa. This allows the representation of values from  $1.175494351\text{e-}38$  to  $3.402823466\text{e}38$ . Thus, the mantissa has a precision of 23 bits which in decimal representation means 7 digits.

The use of single precision for the variables of the position of the particles presents problems in different computations:

# Application of Multiphase SPH to Fluid Structure Interaction Problems

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**Abstract**—This paper presents an alternative formulation of the Smoothed Particle Hydrodynamics (SPH) method applied to Fluid Structure Interaction (FSI) problems involving both single- and multiphase flows. This work extends a pressure-entropy formulation developed for cosmological mixing problems with contact discontinuities, which defines the particle volume without using explicitly the mass density [1]. This formulation eliminates the artificial gap reported at the interface of high-density ratio fluid flows [2, 3], which is a source of instabilities and particle disorder. Our numerical study is performed using a SPH solver that simultaneously models both the fluid dynamics and structural dynamics with a two-way fluid-structure coupling. The coupling is made using the ‘skin’ particle formulation proposed in [4] to ‘wrap’ the solid, thus allowing arbitrary geometries to be modelled. Each component of the method is validated using existing experimental and numerical data. We present results for two benchmark problems: (i) tank sloshing, as in [5], is used to validate the accuracy of the impact load predictions on tank walls considering both single- and multi-phase cases. Also, (ii) flexible gate, as in [6], is used to validate the effectiveness of our FSI coupling in three dimensions. In both cases, good quantitative agreement to experimental measurements is obtained.

## I. INTRODUCTION

In many engineering applications, where fluid and solid motion are of the same order, the dynamics of both media are studied together; this type of analysis is known as Fluid-Structure Interaction (FSI). One of the challenges for numerical simulations of FSI problems with large deformation and nonlinear fluid motion is the assessment of the fluid load acting on the structure, due to its influence in the entire system evolution. In a standard FSI modeling, a Lagrangian formulation is used in the structural domain and a Eulerian formulation in the fluid domain. Both media are coupled using a hybrid formulation to update the structure deformation and remesh the fluid domain at each time step.

In large deformation problems, the computational cost is high because a nonlinear Lagrangian formulation is used and the accuracy of the load estimation decreases since large-aspect cells are generated near the interface in the remeshing process. For this reason, an alternative methodology was used in this work to describe both media in a natural way, in an effort to take advantage of meshfree methods capabilities, such as Smoothed Particle Hydrodynamics (SPH).

SPH uses a set of discrete points carrying a constant mass, thought as particles, to represent the time evolution of a system according to their governing equations [7]. Along the years, it has been used to study several problems involving either fluids or solids only. For example, solid deformation [8], free surface flows [9], multiphase flows [10], wedge water entries [11], fast ship simulation [12], high-speed impact [13], and underwater explosions [14]. However, only few publications of FSI problems have been performed using a full SPH algorithm, given the limitations of the formulation used in the fluid-structure coupling. Reference [6] was the first one to address this, where the calculation of the interface location and its normal vectors is required; which could limit the simulation to concave surfaces and two-dimensional geometries.

In this work, the fluid-structure coupling was made using a ‘skin’ particle layer to ‘wrap’ the solid. These particles exert a repulsive force over fluid particles using a modified version of [4]. This formulation allows to model arbitrary geometries because it is easy to calibrate, the normal vector calculation is not required, and the resulting force is ‘almost’ normal to the surface of the structure.

An additional challenge is the implementation of a multiphase SPH model able to handle high-density ratio flows. Recent works have reported some limitations for this kind of simulations, i.e.: an artificial gap develops at the interface and the requirement to use an artificial pressure gradient force to avoid interpenetration [10] or particle disorder that could lead to instabilities [2]. In this work, an alternative formulation was explored to eliminate these shortcomings. It extended a pressure-entropy formulation developed for cosmological mixing problems with contact discontinuities [1] to high-density ratios flows.

This paper is organized as follows: Section II describes the Pressure-Entropy formulation developed in [1] and the proposed extension to air-water flows. Section III describes the rigid boundary condition for interaction with water and air particles, and the fluid-structure coupling algorithm. Section IV shows validation results for (i) sloshing tank problem considering single-phase and multiphase flow to validate the accuracy of the impact load predictions on tank wall. (ii) Three-dimensional flexible gate problem to validate the

# Drying and Morphology Evolution of Single Droplets in Spray Processes

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**Spray drying is a technique, where solid particles are manufactured from a liquid feed. The product morphology is a crucial property for the further processing. In this contribution we present an SPH model of suspension drying based on first principles, where the underlying physical effects of drying, interaction of the suspended primary particles and surface tension and wetting are considered on a detailed scale. Simulations have been carried out for two-dimensional droplets and show a good agreement with drying theory and experimental findings. The results show a dependence of the final product structure on physical properties like the contact angle or process parameters like the drying rate. A simulation of different drying regimes is possible, too.**

## I. INTRODUCTION

Spray drying is a widely used technique in process industries. A liquid feed consisting of a solution or a suspension is atomised at the top of a heated dryer. As the droplets fall down within the spray dryer, the liquid phase evaporates. The final product is a powder consisting of small, solid particles. Typical applications of this process lie in food industries or in the production of pharmaceuticals as well as in other fields. The morphology of the spray dried particles is a crucial property for the further manufacturing of the product. The evolution of structure within a single droplet is influenced by many different physical effects and still subject to current research [1].

Simulations of the spray drying process have been undertaken in different dimensions. In large scale simulations a whole spray dryer, which in industrial scale may be of up to 15 m height, is considered and simulated by typical mesh-based CFD-techniques [2][3]. The droplets are followed using Euler-Lagrange couplings with the physical processes inside these droplets being implemented by simplified, lumped models. Whereas this approach gives an insight into the process as a whole, single droplet drying models are employed for a more detailed understanding of the interplay of the different physical effects and their effect on the drying process. A thorough review over many of these models has been given by Mezhericher et al. [4][5]. Commonly, a spherically symmetric droplet geometry is assumed. Transport equations inside the droplet can be reduced to the radial direction due to symmetry. Physical phases are expected to be quasi-homogeneous, whereby in suspension drying often a distinction between a porous, solid crust and a wet core is made. The drying curve of a single droplet can be simulated very well by such models, if the physical parameters are adjusted appropriately. However, such parameters are often averaged and tuned to experiments. This kind of models is hence very limited for the

prediction of structure-related properties like the porosity or breaking strength of the crust, as the parameterisation itself already contains implicit assumptions about the product structure. A modelling approach, which accounts for the physical effects during drying on a more detailed scale, is therefore highly desirable. However, modelling the evolution of structure in a multiphase regime is challenging with grid-based methods. In the following, we therefore introduce an SPH drying model, which shall account for structure formation based on first principles.

## II. BASIC EQUATIONS IN DROPLET DRYING AND THEIR SPH COUNTERPART

In this section we will provide a short introduction into typical equations used in single droplet drying models. SPH implementations for transport inside the droplet can be found in the SPH literature. The application of linear driving force boundary conditions, which are commonly used in drying models, is not straightforward in SPH and will be explained more extensively.

### A. Transport inside the droplet

Typically, a diffusion dominated transport regime is assumed inside the droplet. The effect of circular convection due to friction can be assumed to be small in comparison to diffusion [6]. In this contribution, we will not consider solute transport by diffusion, as the suspended solid particles will be modelled in SPH in detail. Hence, only heat transport inside the droplet has to be taken into account. Fourier's second law with respect to the radial direction  $r$  in spherical coordinates is

$$\frac{dT}{dt} = \frac{1}{\rho c_p} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \lambda \frac{\partial T}{\partial r} \right). \quad (1)$$

$\rho$  is the density,  $c_p$  the specific heat capacity,  $\lambda$  the heat conduction coefficient and  $T$  the temperature. With heat conduction being by far the most dominant effect, heat transport by mass diffusion and convection can be neglected. The SPH discretisation is undertaken in Cartesian coordinates and was derived by Cleary and Monaghan [7], who used the Brookshaw formulation for the Laplacian, but a harmonic mean for the average heat conduction coefficient.

$$\left. \frac{dT_i}{dt} \right|_{cond} = \frac{2}{\rho_i c_{p,i}} \sum_j \frac{m_j}{\rho_j} \frac{2\lambda_i \lambda_j}{\lambda_i + \lambda_j} \frac{T_i - T_j}{r_{ij}} \frac{dW}{dr_{ij}} \quad (2)$$

# Pairwise Force Smoothed Particle Hydrodynamics Multiphase Flow Model

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**Abstract**—We propose a novel parameterization of the Pair-Wise Force Smoothed Particle Hydrodynamics (PF-SPH) multiphase flow model and validate it using micromodel experiments. First, we derive analytical expressions relating parameters in the PF-SPH model to the surface tension and static contact angle. Next, we use the model to study viscous fingering, capillary fingering, and stable displacement of immiscible fluids in porous media for a wide range of capillary numbers and viscosity ratios. We demonstrate that the steady state saturation profiles and the boundaries of viscous fingering, capillary fingering, and stable displacement regions compare favorably with micromodel laboratory experimental results. For a displacing fluid with low viscosity, we observed that the displacement pattern changes from viscous fingering to stable displacement with increasing injection rate. When a high viscosity fluid is injected, transition behavior from capillary fingering to stable displacement occurred as the flow rate was increased. These observations are also in agreement with the results of the micromodel laboratory experiments.

## I. INTRODUCTION

In this work we propose a novel parameterization of the Pair-Wise Force Smoothed Particle Hydrodynamics (PF-SPH) multiphase flow model and validate it using micromodel experiments. In the PF-SPH model, the surface tension and wetting behavior of fluids is modeled with pair-wise molecular-like forces. The accuracy and consistency of the PF-SPH model for simulating surface angle and static and dynamic contact angles for flows in domains with simple geometries, such as flat surfaces and fractures with uniform apertures have been demonstrated in a number of papers including [1]–[3]. Here we derive analytical expressions relating parameters in the PF-SPH model to the surface tension and static contact angle.

Traditionally, periodic boundary conditions for fluid pressure and velocity have been used in SPH models, and the flow has been driven by a gravity/body force. In general, two-phase flow is not periodic and periodic boundary conditions cannot be used to describe such flows accurately. Also, in many laboratory experiments the fluids are introduced in a flow cell with a constant flow rate. In the present work, we propose a new method for implementing the prescribed flux boundary condition in SPH.

In general, the displacement behavior in porous media of one fluid by another is determined by the balance between capillary, viscous, and gravity forces. Here we consider a horizontal flow in a two-dimensional porous medium. Such flows

have been studied experimentally using quasi-two-dimensional micromodels, in which (when placed horizontally) the effect of gravity is negligible compared to capillary and viscous forces. The flow displacement in the absence of gravity can be described by two non-dimensional numbers: the capillary number  $Ca = v\mu_d/\sigma$  and viscosity ratio  $M = \mu_d/\mu_r$ , where  $v$  is the average pore-scale velocity of the displacing fluid,  $\mu_d$  is the viscosity of the displacing fluid,  $\sigma$  is the interfacial tension, and  $\mu_r$  is the viscosity of the resident fluid. [4] did pioneering work on studying and visualizing pore-scale displacement phenomenon using micromodels. They established three basic displacement regimes: capillary fingering, viscous fingering, and stable displacement. Viscous fingering occurs at high flow rates (high  $Ca$ ), when a low viscosity (higher mobility) fluid invades a high viscosity (low mobility) fluid and is characterized by narrow forward progressing flow paths. Capillary fingering occurs at low flow rates (low  $Ca$ ) over a wide range of viscosity ratios. Capillary fingering takes place in the form of wide forward and lateral nonwetting phase flow paths. Stable displacement occurs at high flow rates when a high viscosity fluid displaces a low viscosity fluid and has the form of a flat moving front with no fingering behaviors. As  $M$  increases, flow crosses over from viscous fingering to the stable displacement region. As  $Ca$  increases, flow crosses over from capillary fingering to the stable displacement region.

We use the PF-SPH model to simulate displacement of a fluid initially occupying a micro-cell with another fluid injected into the cell at a constant flow rate under a wide range of  $Ca$  and  $M$  numbers. We compare the model results with the experimental results of [5] and [4], who conducted a series of displacement experiments in a micromodel representing a uniform two-dimensional porous medium. We demonstrate that the PF-SPH model is capable of capturing different flow regimes including viscous fingering, capillary fingering, and stable displacement and the transition behaviors. The detailed description of the PF-SPH model and validation study can be found in [6].

## II. PAIR-WISE FORCE SPH METHOD

In the Pair-Wise Force SPH (PF-SPH) method, the momentum conservation equation for each fluid phase is discretized

# Application of SPH method using interparticle contact algorithms to mesomechanics of heterogeneous media

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**Riemann solver for hyperbolic equations and discontinuity breakup solutions for parabolic equations have been implemented in SPH by the authors of this paper. In this approach the SPH equations are written in terms of the interparticle contact values of the dependent variables and fluxes. The improved SPH method is used to solve a number of problems. Simulation of propagation of failure waves in brittle materials and compaction waves in liquid metals with solid metal inclusions is performed. Shock wave compression of porous materials and detonation wave in porous explosive are simulated on the mesostructure scale.**

## I. INTRODUCTION

Numerical methods of solving the equations of dynamics of continuous media used to be the only instrument to discover the processes occurring in heterogeneous media exposed to impact-wave loading. There aren't analytical solutions for these problems. List of heterogeneous media exposed to impact-wave loading is wide enough – ceramics, powder metallurgy materials, space-armed composite materials, structure components of various reactors, foamed materials and explosives with inert additions.

Behaviour of heterogeneous media submerged to dynamic loading is described by various physical models. Porous material, e.g. in the zone of high pressures can be modeled well enough with averaged equations of conservation with effective equations of state, thus the strength, and thermo-physical properties must be defined experimentally. On atomic level the molecular dynamic is a powerful instrument for simulation of cavities under load with high stress in material. But because of limited computational resources molecular dynamics meets the difficulties in modelling the flows in the spatial and temporal scales exist in the experiments. In this paper application of the modified SPH method for various problems of impact loading for condensed matter is presented.

To increase calculation monotonicity and accuracy in the region of contact of two materials with a large difference in physical and mechanical properties, a variant of the SPH method without artificial viscosity based on the solution to the Riemann problem was developed. In [1], [2], this concept was introduced for condensed strength media, and then was applied

to simulate shock waves in heterogeneous media and diffraction of detonation waves in explosives with inert inclusions. The standard SPH method with artificial viscosity and the modified SPH method with Riemann solvers were extensively compared in [1], where accuracy estimates were made for both methods in the vicinity of contact discontinuities and in rarefaction and compression waves.

In this paper the results of simulation of a number of problems in mesomechanics of heterogeneous and reacting media are presented.

Plane failure waves in a brittle material loaded by an elastic compression wave are simulated using the failure model with the measured velocity of propagation of the failure wave and a failure condition of the Drucker-Prager type. Compression of glasses with shock-wave while the stress is being exceeded the threshold value cause the wave of material fracture. It propagates in compressed elastic brittle material with a speed, less than sound velocity and close to the limiting value of speed of fracture growing. The fracture wave has the narrow front, in this front the continuity of the material is being broken as a result of the explosive fracture growing.

The structure of shock waves is simulated in heterogeneous media composed of two components: liquid lithium and solid tungsten inclusions. The problem is solved in thermal viscous elastoplastic 2D formulation. The computations show that the flow in the shock front has characteristic pulsations of temperature and velocity caused by well pronounced temperature and velocity difference between the carrying and inclusion phases. The process of temperature and velocity relaxation determines the width of the shock front.

A mesomechanical simulation of porous aluminum shock loading is performed. The 2D periodic structure of porous material is presented explicitly and the properties of solid aluminum are used. The shock loading is simulated by the impact of a porous plate against a rigid wall. The material flow fields show major features of loading dynamics: multiwave shock structure at low shock intensities, hydrodynamics of the pore collapse in a strong shock and formation of the two-step material compression at the shock front, the generation of pressure oscillations behind the shock front and the influence

# 3-D SPH scheme with variable resolution: assessment of the optimal splitting refinement pattern

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**Abstract**—In this paper a 3-D SPH numerical scheme with variable resolution is presented. The key idea of the algorithm is to use particle splitting and coalescing to modify the particle size according to some criteria. Different 3-D particle splitting stencils have been analyzed by means of the density error minimization procedure and the optimal stencil has been assessed, considering both accuracy and efficiency. The SPH algorithm is variationally derived and this guarantees that both mass and momentum are conserved also when particles with different smoothing lengths are considered. To prevent highly anisotropic distributions of the particles, a generalized shifting procedure which can address also domains discretized with variable mass particles is included. The code has been developed by extending the open source parallel-SPHysics code, and thus can exploit the cluster computing capability.

The algorithm has been tested against Poiseuille and Lid-driven flows showing a good agreement with reference solution.

## I. INTRODUCTION

In mature numerical schemes variable resolution is adopted in order to improve the efficiency of the simulation without reducing the accuracy. In particular in Eulerian schemes different approaches are available in literature such as unstructured grids [5], Adaptive Mesh Refinement (AMR) based on Octree grids [14] etc. Adaptivity is more difficult to achieve in SPH due to the Lagrangian nature of the method. Previous works in SPH have introduced variable resolution by either remeshing, and particle insertion/removal techniques [3], [8], dynamically varying particle characteristics [18], or through variable smoothing lengths with dynamic particle splitting and coalescing according to pre-defined criteria [19], [20]. In the Finite Volume Particle Method multi-resolution by Eulerian particles for high resolution zones [15] has been used. Only recently have schemes appeared that offer both runtime particle splitting and coalescing to provide dynamic adaptive resolution [2], [16], [20]. Feldman and Bonet [4] defined the refinement stencil that should be used for 2-D models, however all those previous works are developed considering 2-D schemes whereas little attention has been dedicated to 3-D. The aim of this work is to develop a 3-D particle refinement scheme that includes both dynamic

particle splitting and coalescing that minimises error within a SPH simulation. In this work the global density error minimization algorithm has been extended to 3-D to define the position, smoothing length and other physical quantities of each daughter particle. Four different splitting patterns have been considered: cubic, cubic with additional particles located in the centre of the faces, icosahedron and dodecahedron. An accuracy analysis of how the daughter particle positions and smoothing lengths affect the global density error and the mass distribution has been conducted for each refinement pattern. Finally the optimal refinement pattern for 3-D simulations is identified. Both the Wendland and the cubic-spline kernels have been used to demonstrate that the analysis is independent of the choice of kernel.

The particle coalescing procedure presented in [19] has been extended to 3-D to reduce the number of particles where high resolution is no longer necessary.

Mass and momentum conservation, also in the presence of particles with variable mass and smoothing length is guaranteed by using a weakly compressible variationally consistent SPH algorithm. The numerical scheme has been developed by extending the capability of the parallel SPHysics open-source software ([www.sphysics.org](http://www.sphysics.org)).

To increase the accuracy a particle shifting correction [17] has been used in the update of the particle position, and an additional diffusion term has been added to the continuity equation [10].

## II. PARTICLE SPLITTING

### A. splitting procedure

To increase the resolution in certain areas of the domain one original particle  $N$  is split into  $M$  daughter particles. The mass  $m_k$ , position  $\mathbf{x}_k$ , velocity vector  $\mathbf{v}_k$ , and smoothing length  $h_k$  for any of the  $k = 1 \dots M$  refined particles must be defined, therefore the total number of degrees of freedom is 8 (in 3-D) for each  $k$ -th daughter particle. To reduce the degrees of freedom of the problem, the number of new particles  $M$



# Particle Filling and the Importance of the SPH Inertia Tensor

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**Abstract**— In this contribution we present an extended version of the Weighted Voronoi Tessellation (WVT) algorithm as a powerful method to generate and improve initial particles distributions [1]. With this method it becomes simple to create distributions of particles of non-uniform size and to fill arbitrarily shaped domains. The possibility to create initial distributions of particles with varying size allows reducing the number of particles and related computational effort while maintaining sufficiently fine particles in regions where high accuracy is required. The quality of the resulting particle distribution for an SPH simulation requires that the particle size varies smoothly throughout the entire domain and that the distribution remains locally isotropic. The equivalent of the inertia tensor for each particle is demonstrated to define an appropriate quantitative measure of the local anisotropy. It will be shown that WVT algorithm is consistent with the requirements for a distribution to be stable under gravity loads.

## I. INTRODUCTION

Application of SPH and other particle methods to practical engineering studies without the need for huge computer resources may significantly be enhanced if it would be possible, by a simple procedure, to generate particles with a fine distribution where required and coarser elsewhere. The resulting particle distribution should be of sufficient quality, a property that will be detailed in this paper. Generating distributions of particles of non-uniform size is not simple since the particles should cover the volume properly i.e. the particle density number should be equal to one at the interior, and there should be no abrupt changes in particle size. If small particles located on top of much bigger particles the smaller particles will migrate through their larger neighbours when subjected to gravity. As will be demonstrated, the above requirements are not sufficient to guarantee that a particle distribution remains stable when subjected to external force fields. In addition, it is required that the particle distribution is ‘isotropic’ in terms of neighbours in various directions. The SPH inertia tensor will be defined as a quantity to assess the isotropy. The ratio of the largest and the smallest eigenvalue of this tensor (anisotropy ratio) may be defined as a scalar quantity that has to be close to one for any particle not near a boundary to warrant stability.

A suitable method for generating particle configurations for optimal initial conditions is the Weighted Voronoi Tessellation (WVT) algorithm proposed by Diehl et al. [1]. This algorithm

has been extended by various options to fill a domain bounded by an arbitrary geometry and by allowing the particles to grow in size while they are filling the domain. It will be demonstrated that an extended WVT (EWVT) procedure allows generating distributions of sufficient quality, with the anisotropic ratio close to one, to be used for SPH flow simulations. Various examples, in 2D and 3D, will be discussed.

The possibilities to use the EWVT to fill a domain of complex shape with particles will also be addressed. Finally, the possibility to enhance the quality of the particle distribution **during** SPH flow simulations using an algorithm based upon the WVT method and thus ameliorating the tension instability, will be discussed.

## II. THE WVT ALGORITHM

### A. Non-uniform particle distributions

A shortcoming of the standard SPH approach is the difficulty to employ a non-uniform volume discretization. For flow simulations such a feature allows using a fine discretization for the regions where this is relevant, as for instance where there is contact with structures. The difficulty is related to the requirement that the particle distribution should locally be sufficiently uniform as well as isotropic and without sudden discontinuities in particle size. If, for example, a rectangular domain is filled with particles placed at equal distance from each other in horizontal directions, but at an increasing distance in vertical (downward) direction, the larger particles near the bottom may have more neighbours in horizontal directions than in vertical direction. Such a distribution may give rise to unphysical flow phenomena. To overcome this problem, the Weighted Voronoi Tessellation (WVT) method originally proposed by Diehl et al. [1] has been implemented in VPS (Virtual Performance Solution).

### B. Overview of the original WVT algorithm

A Voronoi diagram (or tessellation) is a way of dividing space into a number of regions. A set of points (called seeds) is specified beforehand and for each seed there will be a corresponding region consisting of all points closer to that seed than to any other. The regions are called Voronoi cells. It is dual to the Delaunay triangulation. The Delaunay triangulation defines the basis of the Natural Element Method (NEM) of

# Smoothed Particle Hydrodynamics with Adaptive Discretization

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**Abstract**—By combining a local adaptive refinement technique with a newly developed coarsening algorithm, we found a Smoothed Particle Hydrodynamics (SPH) formulation that allows for a dynamic adaptation of the discretization level of a simulated continuum at runtime. With this advanced SPH method, one is able to improve the accuracy of the simulation results while reducing the required computational cost at the same time. For this purpose, the number of particles is, on the one hand, adaptively increased in critical areas of a simulation model, i.e. areas showing a too low particle density. On the other hand, the number of discretization points is decreased in domains of little interest and high particle density. Besides a very brief introduction to the SPH approximation procedure we use to discretize fluid and solid continua, the extensions to the original formalism necessary to provide a truly dynamic model resolution are presented and it is shown in this paper how they can be efficiently implemented. Following this, the applicability of the enhanced formulation, as well as the benefit gained from the adaptive discretization, is demonstrated for several examples.

## I. INTRODUCTION

Most Smoothed Particle Hydrodynamics (SPH) software provides no option for a variable model resolution since there is no convenient and well-established extension making this feature available so far. This is especially a problem when it comes to industrial application of such numerical tools as some of their potential in terms of results accuracy and/or computation time is wasted that way. For this reason, we address this issue and developed an enhanced adaptive discretization strategy for SPH by combining a more sophisticated version of the dynamic particle refinement approach presented in [1] with a newly developed coarsening algorithm. For the development of the coarsening part of the routine, the approach proposed in [2] served as a good starting point, but relies exclusively on a random particle selection strategy and is restricted to pairs of adaptive particles. Therefore, we designed a new, advanced resolution scheme that allows for a merging of a user-defined number of SPH particles and takes into account the refinement history of each adaptive particle. In addition to that, we integrated an algorithm providing an automated refinement of the near-surface areas of a simulation model.

After having introduced the modifications to be made to the classical SPH approximation procedure in order to provide such a local adaptive refinement and coarsening of the modeled structure in the first part of this paper, the applicability of the

proposed formulation as well as the benefit gained from it are demonstrated. To that end, the results of different two- and three-dimensional fluid and solid simulations obtained with the particle simulation package Pasimodo [3] are discussed.

## II. SMOOTHED PARTICLE HYDRODYNAMICS FOR FLUIDS AND SOLIDS

The SPH discretization procedure we use to approximate the well-known Euler equations follows the one proposed in [4]. In case of fluid dynamics, the liquid is assumed to be weakly compressible and, according to this, the exponent  $\gamma$  of the employed Cole equation of state [5] is chosen to be 7. The parameters  $\alpha$  and  $\beta$  of the artificial viscosity term are set to values 0.01 and 0, respectively. The kernel  $W$  is a Gaussian function with an initial smoothing length of 1.5 times the initial particle spacing. For time integration, the second-order explicit Leapfrog scheme [6] is used and the corresponding step size is determined by the Courant-Friedrichs-Lewy condition [7].

In case of solid mechanics, the Mie-Grüneisen equation of state [8] is deployed to close the system of governing equations. Besides, the parameters  $\alpha$  and  $\beta$  are chosen to be 1.0 and 2.0, respectively, the parameter of the artificial stress tensor is set to a value of 0.15, and the initial smoothing length has a value of 1.7 times the initial particle spacing. As some of the simulation scenarios used for the validation of the proposed adaptive resolution scheme show a plastic response of the modeled continuum, the basic SPH solid formulation introduced in [4] needs to be extended accordingly. The modifications made in terms of solid material model, as well as an appropriate force model for boundary interactions, are briefly discussed hereinafter. Detailed information on our enhanced SPH formulation for solid bodies can be found in the 2013 SPHERIC Workshop Proceedings [9].

### A. Plasticity Model

The SPH solid material model can be extended to plastic behavior based on the von Mises equivalent stress  $\sigma_{vM}$ . With the von Mises stress and the yield strength  $\sigma_y$ , a plastic character of the material is identified in the case that the von Mises yield criterion

$$f_{pl} = \frac{\sigma_y}{\sigma_{vM}} < 1 \quad (1)$$

# Toward a higher order SPH-ALE method based on Moving Least Squares method

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**Abstract**—This paper describes the development of a high order meshless method for the solution of weakly compressible flow obtained with a meshless method. The novelty of this approach is based on the use of least squares fitting to compute the state at the interface in the numerical flux reconstruction step. The main principle motivation of this work is to reduce the numerical dissipation in the Riemann solver used to compute numerical fluxes. Numerical simulations show the accuracy and the robustness of the numerical approach for inviscid flows.

## I. INTRODUCTION

Nowadays computational fluid dynamics (CFD) is routinely used for many applications in aerodynamics, hydromechanics and aerospace. Complex geometries are used and favour unstructured grids. The fact of achieving high-order of accuracy in this case remains a great challenge to capture complex flow features. Mesh based methods like high order continuous finite element methods (FEMs), discontinuous Galerkin methods (DGMs) and finite volume methods (FVMs) have gained popularity for the numerical simulation of compressible and incompressible Euler and Navier-Stokes equations. For reasons of robustness and cost of calculation, second-order finite-volume schemes are routinely used for engineering problems. However, for a set of industrial application, mesh-based methods are not always efficient and easy to use (free surface, moving geometries...). An idea was to develop methods where meshes are not necessary.

In 1977, the SPH method (Smooth Particle Hydrodynamics) was discovered by Lucy for astrophysical application. Some years later, a new branch of this classic SPH method was developed by Jean-Paul Vila in 1999 [1] [2] : the SPH-ALE method. The main idea of this last work is to use Riemann solvers to compute numerical fluxes unlike classical SPH approach where an artificial viscosity is used to stabilize the method (Monaghan [13]). Many authors have worked on this meshless method [21] [22] [20] to improve its capacities.

In this paper, we compare two strategies to reduce the numerical dissipation and to increase the accuracy of the numerical results : the first strategy is to use a  $h$ -refinement where the particles radius  $h$  is gradually reduced; the second

possibility is the use of high-order approximation so called a  $p$ -refinement. These both approaches are very popular in the Finite Element method. The pioneer for this idea was Babuska [8]. We can note the paper of Jameson et al [16], where a comparison between  $h$  and  $p$  refinement is presented and shows the possibility of a  $p$ -refinement for smooth flows.

The first key issue in the development of high-order meshless SPH-ALE schemes is the implementation of efficient reconstruction procedures of unknown variables at each interface for each interaction. The numerical dissipation due to the Riemann solver can be reduced with a MUSCL reconstruction (Monotone Upwind Scheme for Conservation Laws) introduced by van Leer in 1979. The idea is to replace the piecewise constant approximation of Godunov's scheme by piecewise linear reconstructed states.

On unstructured meshes, one of the classical ways to obtain high resolution results is to use the  $k$ -exact reconstruction [11] [12] together with a slope limiter. The slope limiter is used to guarantee the monotonicity of solutions. The first implementation in this framework of a limiter function was by Barth and Jespersen [10]. Another way to do a scattered data approximation, and very famous in the meshless community is the use of Moving Least Squares (MLS) method proposed by Lancaster and Salkauskas [4] for smoothing and interpolating data in 1981. This method is based on minimizing a least squares functional with respect to the nodal parameters. A lot of research use this latter technique : in the field of meshless methods one can cite Dilts [15] or Afshar et al [18] and in the field of unstructured Finite Volume search one can cite S.Khelladi : [6] [7]. Other alternative approaches were developed, a hybridization between WENO methods and MLS approximation was published [19] to improve the accuracy of the SPH-ALE method for compressible flow. We can cite other works based on the radial basis function (RBF) with A. Iske (2000) [14].

In the frame of SPH-ALE method, to show the ability of the  $p$ -refinement, we propose to test the  $k$ -exact reconstruction and the MLS approximation. We will compare these reconstructions with the historical approach ( $2^{nd}$  order

# Flow Structure Detection with Smoothed Particle Hydrodynamics

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**Abstract**—We discuss how existing flow structure detection methods can be realised in Smoothed Particle Hydrodynamics (SPH) simulations. We demonstrate the use of the  $\Delta$  criterion for the detection of instantaneous Eulerian flow structures. The standard calculation of the velocity gradient tensor (VGT) results too noisy gradient field. We propose a correction method based on the idea of XSPH that yields a much smoother VGT field, enabling significantly more accurate structure detection. We also demonstrate on test cases the process in which the instantaneous Eulerian tools are used to locate Lagrangian coherent flow structures.

## I. INTRODUCTION

Finding reliable algorithms to pinpoint a flow structure in the data of a sizable computer simulation has become a key issue in most fields of computational fluid dynamics. The different flow structure identification methods can be roughly classified as Eulerian or Lagrangian.

Eulerian methods operate on the instantaneous flow field and treat it as if it was steady. This is a serious drawback with respect to Lagrangian ones that try to capture the flow features evolving in time. However, the computational demands on resources has so far prevented the latter ones from becoming routine analytic tasks. The best approach seems to be the application of an appropriate Eulerian criterion at some time to the instantaneous fields to capture *candidates* of Lagrangian flow structures. Having narrowed down to a much smaller part of the fluid, high demand calculations can be started to further verify or exclude the existence of Lagrangian flow features.

An important goal of the Eulerian methods is to detect vortices, and, therefore, a great number of methods have been developed for that purpose. Unfortunately, the very meaning of a vortex is unclear: high vorticity and circular motion, the main characteristics of a vortex, do not necessarily coincide, like e.g. in shear layers. It seems that as many definitions of vortex exist as many vortex detection algorithms. Instead of seeking for a good definition of a vortex, one may look for a good vortex detection algorithm instead. Apart from practical issues three principal requirements have been formulated: a good algorithm has to be dimensionless [1], frame-independent [2] and capable of describing compressible fluids [3].

The last point seems to be the most decisive from the point of SPH, which is, by design, compressible — at least weakly. Therefore in Section II, following the recommendations of [3],

we present the concept of the  $\Delta$ -criterion (which also happens to be Galilean invariant) for two and three dimensional SPH applications. Another key issue is whether it is possible to achieve such a precision in SPH that the spatial derivatives of the velocity field necessary for the Eulerian criteria can be calculated: this problem will be discussed in Section III.

Finally, in Section IV, we shall turn to the investigation of Lagrangian flow structures. As SPH is a genuine Lagrangian method, the field variables are related to particles in the material frame. This makes SPH a very promising potential tool for Lagrangian structure detection problems. The central notion in the Lagrangian problems is *mixing*: certain types of Lagrangian coherent structures are defined as the ones that maintain their identity, other types correspond to barriers to material transport. We calculate two quantities that characterize the local strength of mixing in suspected Lagrangian coherent structures: relative dispersion and finite time Lyapunov exponents (FTLE).

The computations we present have been carried out by our parallel SPH solver written in CUDA and C++.

## II. THEORETICAL BACKGROUND

### A. Flow Structures and Dynamical Systems

The flow pattern of *steady flows* can be completely described by the local analysis of their stagnation points and the global analysis of their invariant manifolds [4]. Due to the achievements of dynamical systems' theory this seems to be a closed problem, even if in specific cases the actual computations can be challenging.

The simplest case is that of isochoric (divergence free) steady plane flows; their most typical flow features are

- two types of stagnation points — elliptic (centres) and hyperbolic (saddles) points —,
- elliptic islands containing closed streamlines, which loop around the centres, and
- separatrices — stable and unstable invariant manifolds of the saddles — that form boundaries among the elliptic islands and regions of unbounded flow.

It is natural to identify elliptic islands with vortices and elliptic stagnation points with vortex centres. There is an immediate relation between these (in fact Eulerian) flow structures to the

# Large eddy simulation with SPH: Mission impossible?

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**Abstract**—The goal of this paper is to perform a Large Eddy Simulation using the Smoothed Particle Hydrodynamics method with the unified semi-analytical wall boundary conditions. Before this simulation is presented the Taylor-Green test case with an analytical solution is revisited from a different perspective than usually. Namely, to investigate the capability of SPH to convert momentum from one to another direction in turbulent flows. It will be shown that to obtain adequate results a significant resolution is required.

The Large Eddy Simulation presented in the following shows poor agreement with the established reference data and it will be shown that this can be traced back to resolution issues. Tying this together with the results from the Taylor-Green vortex it can be shown that to perform such simulations the Smoothed Particle Hydrodynamics method needs significant modifications.

## I. INTRODUCTION

In the past year the authors presented a quasi Direct Numerical Simulation (DNS) of a turbulent wall bounded channel flow [1] using Smoothed Particle Hydrodynamics (SPH). The results showed a reasonable agreement with the reference data. The only exception were some numerical discrepancies close to the wall. The channel that was chosen for this simulation was geometrically small in order to reduce the computational demand. Even then, due to the computationally expensive nature of SPH with its large number of neighbours the simulation consumed significant resources on a BlueGene Q supercomputer.

In order to perform this DNS successfully the unified semi-analytical wall boundary conditions by Ferrand *et al.* [2] were utilized. As they enable the correct imposition of wall shear stresses they were an integral part of the simulation. A volume diffusion term was used that was originally introduced by Ferrari *et al.* [3] and modified by Mayrhofer *et al.* [4] in order to reduce numerical density fluctuations. Furthermore, to simulate a 3-D flow, the extension by Mayrhofer *et al.* [5] was used in order to compute the wall normalization parameter. This SPH variant will be presented in greater detail in Section II.

After explaining the background for the simulations to follow,

the Taylor-Green vortex is introduced. This well-known test case consists of a lattice of counter-rotating vortices for which an analytical solution is available [6]. This test case is often used to analyze the stability of a SPH method [7]. In the present context a different aspect of this test case will be highlighted that concerns the resolution requirements for an accurate prediction of the forces in the first time-step. As this test case features periodicity in all directions no boundary is present and thus the results can be treated independently of the boundary model used.

In Section IV an attempt is made at performing a Large Eddy Simulation (LES) of a turbulent closed channel flow. The case is introduced in detail showing that the geometry is significantly bigger than the one used for the DNS in [1]. It is briefly remarked how the values of the simulation are interpolated back to an Eulerian grid in order to extract the necessary statistics to compare to established Eulerian codes. The results show that SPH fails to predict the correct average velocity, which will be tied together with the results presented in Section III.

## II. THE UNIFIED SEMI-ANALYTICAL BOUNDARY CONDITIONS

The unified semi-analytical wall boundary conditions for SPH were first introduced by Kulasegaram *et al.* [8], then improved by Ferrand *et al.* [2]. The basic idea is to replace the standard SPH interpolation procedure by one renormalized by an analytical term  $\gamma$ , *i.e.*

$$[f]_a = \frac{1}{\gamma_a} \sum_{b \in \mathcal{P}} V_b f_b w_{ab}, \quad (1)$$

where  $\mathcal{P}$  is the set of all particles,  $V_b$  the volume of particle  $b$  and  $w_{ab}$  the kernel function as function of the distance vector  $\underline{r}_{ab} = \underline{r}_a - \underline{r}_b$  between particles  $a$  and  $b$ . Furthermore  $f$  is an arbitrary scalar or vector function and  $[f]_a$  is the interpolated value of  $f$  at position  $\underline{r}_a$ . Throughout this paper the fifth-order Wendland polynomial is used which is given by

$$w(r, h) = \frac{\alpha}{h^3} \left(1 - \frac{r}{2h}\right)^4 \left(1 + \frac{2r}{h}\right), \quad (2)$$

# 2D Turbulence Using the SPH Method

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**Abstract**—In this paper we extend our previous study of turbulence in two dimensions using SPH [27]–[29]. The crucial role of the solid no-slip boundaries as sources of vorticity filaments, which significantly affects the flow evolution, has been revealed in laboratory experiments and numerical flow simulations [8]. Keeping this in mind, we use mechanical stirrers moving on specified trajectories as the source of time-dependent forcing to generate turbulence. This is applicable for many industrial and engineering problems in which the sources of turbulence are physical mixers or stirrers.

Our weakly compressible SPH model has been improved using density diffusive term in the continuity equation and using three layers of boundary force particles to model the solid boundaries. The accuracy of the developed model is confirmed by recovering the results of oscillating cylinder flow.

In addition, the ability of the SPH method in simulating the periodic and no-slip boundaries in turbulence driven by either stochastic forces or physical stirrers is studied. The comparison of kinetic energy spectra, vorticity and velocity structure functions and the probability distribution functions with theoretical, experimental and numerical results shows satisfactory agreement.

## I. INTRODUCTION

The results for a stochastic stirrer driving two-dimensional flow in a square container with no-slip boundaries have been conveniently summarised by Van Heijst et al. [8]. The key features are these: the forced turbulence has strong anisotropy and nongaussian statistics; the motion is dominated by a large circulation cell that breaks up then reforms in a process that is repeated; the breakup is associated with a change in angular momentum and kinetic energy and the associated production of enstrophy near the wall. The formation of a large circulation cell in both decaying and driven turbulence with no-slip boundaries distinguishes it from turbulence in doubly-periodic domains as does the anisotropic flow and enstrophy production near the boundaries.

In the present case, where we consider the stirring produced by either a cylinder moving in a two dimensional fluid within a container with no-slip boundaries or with periodic boundaries, or by using stochastic forces to generate turbulence in the same geometry. There are some significant differences between the cylindrical stirrer and the stochastic case. The cylindrical stirrer leaves a wake of vortices, and therefore enstrophy, with a length scale approximately the diameter of the cylinder. These vortices subsequently interact with themselves and with the moving cylinders and with vorticity produced on the

boundaries of the container. The length scale of the vortices initially increases but there is an upper bound to the length scale because the cylinders cut through any very large vortex. We therefore do not expect the large circulation cell seen when a stochastic stirrer is used in a confined container.

The numerical method we use is the particle method SPH. Other methods could be used but we intend to extend our results to problems where breaking waves or disturbed interfaces are produced and, for these problems, SPH has the advantage of being simple to implement while retaining satisfactory accuracy. Furthermore the SPH method has also been used in recent studies of decaying turbulence in two dimensions (Robinson and Monaghan [24], Monaghan [18], Valizadeh and Monaghan [27]) which show that the SPH simulations converge and give results in good agreement with experiments and direct numerical simulations. SPH has also been used in numerous problems involving bodies moving in fluids. These include moving bodies impacting the surface of a fluid (Monaghan and Kos [20], Monaghan et al. [21]), and linked bodies moving through a fluid (Kajtar and Monaghan [9], [10]). The accuracy of the vortex generation was tested by simulating a cylinder that generates vortices as it moves harmonically in a container with periodic boundaries. Our results are in good agreement with those of Dütsch et al. [5].

An issue that has plagued SPH simulations is the way boundary conditions are implemented. In this paper we consider two methods. The first of these is an improved boundary force method (Monaghan and Kajtar [10]), and the second is the method of Adami et al. [1]. The boundary force method has been improved by altering the arrangement of the boundary force particles so that they mimic a material boundary more effectively, and by including weak diffusion in the continuity equation. The density diffusion ensures that the irregular density seen even in systems that have been damped to equilibrium, for example static fluid in a tank, is removed and the results greatly improved [29]. The use of slight diffusion in the continuity equation also improves the method of Adami et al. [1]. The two methods were used for the oscillating cylinder test case and the comparison shows that the results of the two methods agree closely. Because of the flexibility of the boundary force method we use it for the main applications of this paper having in mind further applications that involve bodies breaking through free surfaces.

The principal diagnostic tools we use are the kinetic energy

# Energy conservation in the $\delta$ -SPH scheme

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**Abstract**—An in-depth analysis of the energy conservation in the  $\delta$ -SPH model has been carried on. In comparison to the standard SPH scheme, the mechanical energy equation of the  $\delta$ -SPH variant is characterized by a further term that is generally dissipative and is related to the diffusive operator inside the continuity equation. The behaviour and the structure of such a term have been studied in detail and a number of specifically conceived test cases has been considered, highlighting that the dissipative term is generally small and it mainly acts when spurious high-frequency acoustic components are excited.

## I. INTRODUCTION

The  $\delta$ -SPH scheme is a variant of the standard SPH model that includes a diffusive term in the continuity equation to reduce the high-frequency spurious oscillations in the pressure field. This scheme satisfies the conservation of mass and of the linear and angular momenta and, since its definitions (see [1], [2]), it has been successfully applied to several hydrodynamics problems (see [3]–[6]). In the present work we add a further contribution to the analysis of the  $\delta$ -SPH scheme and study the conservation of energy in such a model.

We show that, in comparison to the standard SPH model, the mechanical energy equation of the  $\delta$ -SPH scheme contains a further term that is generally dissipative and that derives from the diffusive operator inside the continuity equation. Further, we describe the general structure of such a term (hereinafter called diffusive power term) and, through numerical test cases, we draw a qualitative description of its behaviour. Specifically, we considered two test cases where the fluid is inviscid and no solid boundaries are present. Under these hypotheses, it is possible to focus on the evolution of the diffusive power term, neglecting viscous and fluid-body interactions. We observed that the magnitude of the diffusive power term is generally small and it mainly acts during the generation of shock waves or when spurious high-frequency oscillations characterize the pressure field. Since the diffusive power term principally drags energy from the compressible components of the SPH, the  $\delta$ -SPH scheme appears to be somehow “less compressible” than the standard SPH.

The paper is organized as follows: section §III introduces the  $\delta$ -SPH scheme and section §IV describes the main energy terms, the energy equations and define the diffusive power term. Then, sections §V and §VI show some applications of the  $\delta$ -SPH to inviscid free-surface flows and describe the behaviour of the diffusive power term.

## II. THE STANDARD SPH

Hereinafter we call standard SPH the following system:

$$\left\{ \begin{array}{l} \frac{d\rho_i}{dt} = - \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} m_j, \\ \frac{d\mathbf{u}_i}{dt} = - \sum_j \left( \frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla_i W_{ij} m_j + \mathbf{f}_i + \\ \quad + \mu \sum_j \pi_{ij} \nabla_i W_{ij} \frac{m_j}{\rho_j \rho_i} \\ \frac{d\mathbf{r}_i}{dt} = \mathbf{u}_i \quad p_i = c_0^2 (\rho_i - \rho_0) \end{array} \right. \quad (1)$$

where  $\rho_i$ ,  $p_i$  are respectively the density and the pressure of the  $i$ -particle while  $\mathbf{r}_i$  and  $\mathbf{u}_i$  are its position and velocity. The particle mass,  $m_i$ , is constant during the motion so that the global mass is conserved exactly. Here,  $W_{ij}$  is the kernel function (a Wendland kernel is used hereinafter),  $\nabla_i$  denotes the differentiation with respect to  $\mathbf{r}_i$  and  $\mathbf{f}_i$  is the body force at the position  $\mathbf{r}_i$ . Finally, symbols  $\rho_0$  and  $c_0$  indicate the density along the free surface (which is the reference value for the density field) and the sound velocity (assumed to be constant). The dynamic viscosity is indicated through  $\mu$  while the kernel of the viscous term is given in [7] and reads:

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

where  $K = 2(n+2)$  and  $n$  is the number of spatial dimensions.

## III. THE $\delta$ -SPH SCHEME

The  $\delta$ -SPH has been first defined in [1] and further inspected in [2]. It reads:

$$\left\{ \begin{array}{l} \frac{d\rho_i}{dt} = -\rho_i \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_{ij} V_j + \delta h c_0 \mathcal{D}_i \\ \frac{d\mathbf{u}_i}{dt} = -\frac{1}{\rho_i} \sum_j (p_j + p_i) \nabla_i W_{ij} V_j + \mathbf{f}_i + \\ \quad + \frac{\mu}{\rho_i} \sum_j \pi_{ij} \nabla_i W_{ij} V_j \\ \frac{d\mathbf{r}_i}{dt} = \mathbf{u}_i \quad p_i = c_0^2 (\rho_i - \rho_0) \end{array} \right. \quad (3)$$

# An interface-energy conserving approach for the coupling of smoothed-particle-hydrodynamics and finite-element methods for transient fluid-structure interaction

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**Abstract**— The purpose of this work is to present an interface-energy-conserving coupling strategy for transient fluid-structure interaction. The proposed coupling strategy is synchronized and partitioned while handling different time integrators for each subdomain. By imposing the interface's normal velocity continuity, the proposed coupling method guarantees that neither mechanical energy injection nor dissipation will occur at the interface, thus ensuring the coupling simulation's stability over time. Additionally, the numerical simulation will converge in time with the rate of convergence of the worst time integrator chosen for each subdomain.

## I. INTRODUCTION

Fluid-Structure interaction effects are a recurrent issue in many types of multi-physics problems in academic researches as well as in engineering sciences. Several types of numerical approaches exist to investigate this particular phenomenon and allow for more reliable conceptions that help prevent unexpected disasters.

The purpose of the present paper is to present a partitioned coupling approach for fluid-structure interaction involving different time integrators for each sub-domain [1,2,3]. The physical characteristics of the fluid take into account a weakly compressible model. As for the solid structure, non-linear behaviors such as large deformations and plasticity are considered.

The key feature behind the proposed coupling method is the conservation of mechanical energy at the interface that is ensured at each time step. This condition is implemented by means of a weak space-time velocity condition imposed in the normal direction within the contact zone between the solid elements and the fluid particles. Thanks to the fact that neither energy dissipation nor creation takes place at the interface, preservation of numerical stability is assured. Additionally, this condition allows for the minimal convergence order of the time integrators used in the different subdomains to be

conserved.

In this study, a hybrid mesh-less formulation is used to describe fluid particle motion, the SPH-ALE method, proposed by Vila [4]. This method combines the flexibility of the classical Smoothed-Particle-Hydrodynamics method, with the adaptability offered by the Arbitrary-Lagrangian-Eulerian technique in terms of particle free-surface flows tracking. Concerning the solid structure, a finite-element Lagrangian approach is implemented. In order to allow for a simplified tracking of the fluid-structure interface, the SPH-ALE method is used in a Lagrangian framework for the fluid particles (arbitrary velocity is set equal to the fluid velocity).

In terms of coupling strategy, a partitioned but synchronized method is used. Although the choice of applying this type of method, as opposed to a more stable monolithic method, might seem contradictory given the main goals of the proposed coupling technique, it was a necessary choice since monolithic methods can become quite difficult to handle if the fluid and structure are described by very different solvers. By solving a system of coupling equations, synchronization is assured at each time step between the fluid and solid solvers thus helping to avoid typical instability issues inherent to partitioned couplings.

The current paper is organized in a straightforward manner presenting the key stages underlying the development, implementation and validation of the proposed method. Section II and section III focus on presenting the equations and numerical methods governing the fluid and solid subdomains. The coupling strategy and algorithm will be detailed in section IV. Finally section V presents one-dimensional and two-dimensional validation tests verifying the proposed method's robustness and enhanced numerical stability when compared to other partitioned methods currently used.



# Coupling of a SPH-ALE and a Finite Volume Method - Extension to 2D and 3D

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**Abstract**—This paper presents a multidimensional extension of the coupling of Smoothed Particles Hydrodynamics - Arbitrary Lagrange Euler (SPH-ALE) with a mesh-based Finite Volume Method (FVM) that was first presented at last year's SPHERIC workshop [1]. The approach allows us to combine the flexibility of the meshless method SPH-ALE with the advantages of the FVM as for example the well-established boundary treatment and the possibility of anisotropic refinement. The algorithm is very flexible and uses a decomposition of the computational domain into regions where the fields are computed by the FVM, regions where they are computed by SPH and overlapping regions where the information is transferred from FV to SPH and vice versa. The method can be used for fixed SPH particles, particles in Lagrangian motion or particles that move arbitrarily (ALE). FV cells are added in areas where a more accurate (refined) simulation is needed or in regions where there are other advantages to use FVM, as for example at the outlet of the computational domain. In the overlapping region, boundary values for the FV domain are obtained by interpolation from the SPH particles, similar to the CHIMERA method of overlapping grids, while FV cells are used as SPH neighbours for the coupling. For validation the results of two dimensional inviscid academic testcases are presented, the Taylor-Green vortices and the flow around a symmetric NACA hydrofoil.

## I. INTRODUCTION

Due to increasing computing power the Lagrangian method Smoothed Particle Hydrodynamics (SPH) is more and more used for industrial applications in the last years. Especially for free surface flows with moving geometries like for example the flow in the runner of hydraulic Pelton turbines [2], the use of SPH or variants of SPH is advantageous compared to traditional meshbased numerical methods. But also for internal flows without free surfaces there are applications where SPH has great potential because of its meshless nature that treats geometries moving in a complex way without remeshing or mesh interfaces.

However, there is one important drawback of the SPH method. It is difficult to have non-constant particle sizes, i.e. particle refinement is complicated for particles in Lagrangian motion, in particular, anisotropic refinements. SPH is an intrinsically isotropic method with isotropic particles and a kernel function with an isotropic support but flow phenomena often necessitate fine space discretization only in one direction. Close to solid walls for example many particles are needed in

direction normal to the wall but not tangential to the wall. In Finite Volume methods (FVM) long thin cells are used in this region that can be more than ten times longer as large. In the past, some work has been done to develop anisotropic kernel functions for SPH [3], [4] but this is not the approach that this work takes.

We present a flexible coupling method of SPH-ALE with FVM [1] that allows us to refine anisotropically in space and to benefit of the other advantages of mesh based methods like imposing open boundary conditions more easily.

Even if SPH is a meshless method, there are important similarities with FVM, especially in the case of SPH-ALE. Hence, it suggests itself to adapt approaches to SPH that were first developed for FVM. In the 1980s the bottleneck of meshbased methods applied to industrial problems was the mesh generation and multidomain methods were developed to make it possible to subdivide the computational domain into subdomains where the mesh can be created independently. One family of these methods is called CHIMERA methods and uses overlapping meshes where information is transferred from one mesh to the other by interpolated boundary values [5]. In general these methods are very robust but not conservative but for the case where conservative interpolation methods are employed. Then Pärt-Enander showed in her PhD thesis [6] that conservative interpolation methods that interpolate the fluxes instead of the physical field variables [7] are not stable.

In recent years several authors started working on a coupling of SPH with FVM, often inspired by the CHIMERA methods. In 2001 Mancip [8] developed a conservative coupling method for FVM on overlapping meshes that no longer interpolates boundary values for each domain like it is done with CHIMERA methods but uses a smooth coupling function instead. An application of this method to the coupling of SPH and FVM is shown but it necessitates the computation of an approximative mesh for the SPH particles in the overlapping region. At SPHERIC 2013 in Trondheim (Norway) coupling methods of SPH and FVM were presented that are similar to the one presented here. Barcarolo [9] showed a SPH refinement and derefinement procedure as well as a coupling with a Voronoi FVM. Bouscasse [10] and his team developed a multi-purpose interface for coupling SPH with other solvers,

# Coupling between SWASH and SPH for real coastal problems

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**Abstract**—Modelling the whole process of wave propagation, wave transformation and wave-structure interaction is a challenging task both in physical and numerical models. Nevertheless, it is often required for a proper assessment of coastal safety and design of coastal defences. However to study the wave propagation from deep ocean to nearshore is difficult using a single model because multiple scales are present both in time and in space. The present study proposes the use of two different models to generate and propagate the wave field from offshore to nearshore locations. The work aims to develop a technique for the assessment of the action of sea waves on the coast starting from predicted incident wave conditions offshore. Hence a hybrid method has been developed that couples the capabilities of a wave propagation model, SWASH, and a meshfree particle method, DualSPHysics.

## I. INTRODUCTION

The latest decades saw a huge development of numerical modelling applied to real life problems. In coastal engineering in particular, the role of numerical models is increasing as essential alternatives or complementary tools to laboratory experiments and prototype measurements. Numerical models are nowadays often used to assess the processes of wave propagation, wave transformation and wave interaction with coastal structures. However outstanding differences exist between the different kinds of models. For instance, grid-based models are widely used in engineering but they are not suitable to represent violent phenomena characterised by large deformations, whereas meshfree models can be still computationally too expensive. In terms of base equations, Boussinesq or nonlinear shallow water equation models have limitations due to the approximation of the governing equations, meanwhile Navier-Stokes based methods can model properly the physics of fluid hydrodynamics but are still characterized by high computational costs. Thereby a single model capable to represent the wave phenomena that occur both offshore and nearshore and to provide accurate results in reasonable computational times is still a challenge nowadays. A different approach can cope with these drawbacks. If the main scope of the modelling is to represent the entire domain

from the deep ocean to the nearshore region and to characterise the wave propagation and wave interaction with coastal defences and beaches, the coupling between two different numerical models seems to be a reasonable solution. A coupling, or hybridisation technique, between two models characterized by different capabilities and different computational costs can help to get a complete representation of phenomena at stake.

A hybrid method has been developed starting from the wave propagation model SWASH and the meshfree particle method DualSPHysics. The hybrid model has been validated with physical model data. The purpose is to represent and analyse the transformation of the sea waves due to the processes typical of the surf and swash zones, such as shoaling, wave breaking, uprush and backwash, run-up, etc... A proper representation of the waves nearshore will make possible the proper modelling of the interaction between sea waves and coastal defences (sea dikes, breakwaters, embankments) with a particular focus on the extreme storm conditions propagating from offshore and non-linear wave transformation.

The so-called SWASH model has been chosen to propagate the sea waves. SWASH is a time domain model for simulating non-hydrostatic, free-surface and rotational flow. Wave propagation models as SWASH have been proven to be able to simulate accurately surface wave and velocity field from deep water and with satisfactory results both at open ocean and nearshore but they are not suitable to deal with abrupt changes of shape of coastal structures.

An SPH-based model has been used to study the wave transformation and breaking at detailed scale close to the shoreline. DualSPHysics [1] is an open-source numerical model based on the Smoothed Particle Hydrodynamics method and can be freely downloaded from [www.dual.sphysics.org](http://www.dual.sphysics.org). The expensive computational cost of SPH in comparison with other meshbased methods for CFD problems can be partially alleviated by general-purpose graphics processing unit (GPGPU) where a graphics processing unit (GPU card) is used to perform computations traditionally managed by big cluster machines with thousands of CPU cores. Thereby DualSPHysics was designed from the outset to use SPH for real engineering problems with software that can be run on

# Modeling and validation of guided ditching tests using a coupled SPH-FE approach

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**Abstract**—Oblique water impact of structures with high horizontal speed is investigated using a coupled Smoothed Particle Hydrodynamics – Finite Elements (SPH-FE) approach. The paper introduces the topic of aircraft ditching analysis, comprising its necessity together with current challenges. A brief overview of an extensive experimental campaign of guided ditching tests carried out in the FP7-SMAES project is given. Numerical simulations of these tests have been conducted by hybrid SPH-FE models. Key code improvements relevant for state of the art ditching simulations such as translating periodic boundary conditions and spatially non-uniform initial particle distributions using weighted Voronoi tessellation will be presented. Comparison with experimental data in terms of force and strain results is established with the aim to validate the numerical model. Good correlation could be proven for test cases with purely elastic as well as elastic-plastic aluminum panels.

## I. INTRODUCTION

Emergency landing on water (ditching) needs to be studied during aircraft design and certification processes for aircraft certified for extended overwater operations. Hence, it applies for the majority of, if not all, passenger and military aircraft.

The analysis of ditching in research and industry tends towards the (supportive) use of numerical simulation tools [2, 3, 5, 26] due to a number of limitations and drawbacks related to experimental testing which — besides comparison to aircraft with similar design having previously passed ditching certification — is the state of the art means to proof ditching capabilities [5, 22, 24, 31]:

- extensive financial and temporal efforts of test campaigns,
- testing of full-scale aircraft is economically unfeasible,
- inherent but undesirable scale effects in hydrodynamics of sub-scale experiments,
- reduction to rigid sub-scale models, which do not accurately account for deformation and hydroelasticity,
- limitations in terms of design changes and amount of scenarios to be tested,
- limited amount of measurable results (virtually it is possible to display results in manifold ways), etc.

There is a variety of semi-analytical methods utilized to simulate water impact, e.g. [25, 30]. However, when regarding highly non-linear structural behavior with potential failure of complex and realistic structures, semi-analytical approaches

are no longer suitable to solve this fluid-structure interaction problem and advanced numerical methods are needed.

The violent nature of a ditching event, which includes large fluid deformations and complex free surface shapes, identifies the Smoothed Particle Hydrodynamics (SPH) method as well suited for the solution. In order to analyze the structural response including deformation and potential damage, a coupled approach of SPH and the Finite Element (FE) method is chosen.

Challenges for the numerical simulation arise from sharp gradients with extremely small time and spatial scales, which require a relatively fine spatial resolution. Additionally, the fluid domain has to extend far enough beyond the projected area of the impacting structure and also to a sufficient depth to avoid the influence of reflected waves from the numerical boundaries on the interaction with the structure. The resulting number of fine particles required to model a ditching event would become prohibitively large for practical applications to study multiple ditching scenarios or for design purposes. Therefore, the development and enhancement of appropriate numerical simulation tools is required to overcome current limitations. Moreover, reliable experimental data are needed to allow for validation and to enhance the understanding of the involved physical phenomena.

## II. EXPERIMENTAL CAMPAIGN

Water impact experiments of simple geometrical shapes at high horizontal velocity were widely conducted by researchers in the 1940s and 1950s, e.g. [7, 8, 28]. Available results, however, lack a reasonable time resolution and appropriate detail to support code development and essential validation. Therefore, a new experimental campaign of guided ditching tests was conducted, aiming to provide detailed experimental data, i. e. information about the structural loads and deformation as well as pressure distributions at suitable time resolution. Moreover, due to the number and complexity of the physical processes relevant for ditching (which cannot be scaled accurately in sub-scale experiments) full-scale structures at representative impact velocities are used.

# Momentum conserving methods that reduce particle clustering in SPH

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## Abstract

In this paper we present two remedies for particle clustering in SPH. Since particle clustering is the consequence of a diminishing kernel gradient for small inter-particle distances, the first method uses a convex kernel with a non-zero kernel gradient at the origin. The second method is based on inter-particle collisions. They are both compared with conventional SPH in several case studies. The results show a great improvement in particle distribution, where particle clustering is strongly reduced or absent, with only a small influence on the accuracy of the computations.

## I Introduction

One of the unsolved problems in SPH is the pairing, or clustering, of particles. This process in some situations mimics physical processes and fragmentation, making it hard to detect as a numerical artifact [18]. Particle clustering reduces the resolution of the simulation. This not only endangers the accuracy of the results, it is also a waste of computational effort. It is thus of great importance to reduce the numerical clustering of particles as much as possible.

In the battle against particle clustering there is confusion about what is causing the particles to cluster. This confusion is caused by the presence of two types of particle clustering. On the one hand there is an instability known as the tensile instability [14, 18]. This instability can be present in simulations that allow for a negative pressure, but it is also known to occur in problems where the pressure is always positive [14]. SPH particles being subjected to a compressive/tensile stress will repel/attract each other, just like real particles, e.g. atoms, would do. However, in the case of tensile stress this leads to an instability where particles cluster.

On the other hand, there is an instability usually known as the pairing or clumping instability. This instability has little to do with the sign of the stresses, instead it is caused by a diminishing repelling force for approaching particles. Because the gradients of the most commonly used kernels tend to zero for small inter-particle distances, the forces or accelerations calculated from the

momentum equation will also tend to zero. This makes that particles cannot get away from each other. This is the type of instability we consider in this paper. To avoid any confusion regarding the tensile instability we will not use the word ‘instability’, rather we will speak about ‘particle clustering’.

In [3] it is argued that not the diminishing kernel gradient is causing the clustering, but it is in fact caused by a (partly) negative Fourier transform. Since Wendland kernels are constructed to have a positive Fourier transform, they should not suffer from particle clustering. This statement does not agree with our results, as can be seen in Figure 1. The left picture shows the initial situation of a box with periodic boundary conditions. The box is filled with air and all particles have the same mass and are randomly distributed. From a gas we expect that over time it distributes itself more or less uniformly over the domain. However, in the second picture, for which we used the Wendland kernel:

$$W(R) = \alpha_d \begin{cases} (2 - R)^3 \left(\frac{3}{2}R + 1\right) & R \leq 2, \\ 0 & R > 2, \end{cases} \quad (1)$$

the particles are not distributed uniformly over the domain, but are even forming clusters. For more details we refer to Section V.I. Thus also with Wendland kernels particle clustering can occur,

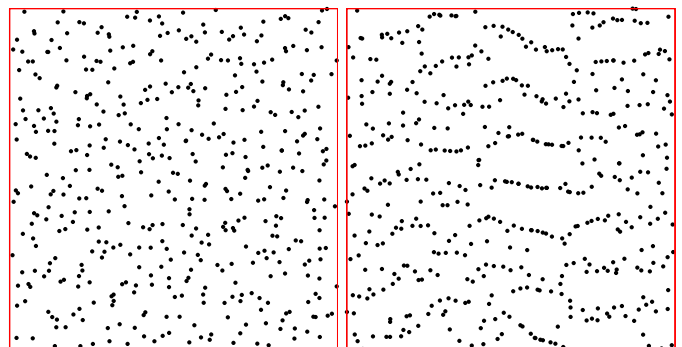


Figure 1: **Particle clustering in action.** The left picture shows the initial configuration. The right picture shows the results when the Wendland kernel as in (1) is used. The clustering of particles is clearly visible.

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# Pressure evaluation improvement for Euler Isentropic SPH scheme

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**Abstract**—One classic drawback of weakly compressible SPH method is the noise in evaluated pressure field. In this paper we present a new set of diffusive term method based on an approach initially introduced by Grenier *et al* [8] in the framework of finite volume method. We extended this approach to SPH approximation.

## I. INTRODUCTION

The SPH method enjoys the advantage of being a meshless, adaptative, Lagrangian method naturally handling discontinuities and free-surfaces [7]. Initially developed by Lucy, Gingold and Monaghan, for astrophysical problems [6], [12], it has been extended to cover the behavior of solids and fluids and, because of its nature, it is able to handle complex phenomena and complicated flow patterns, without having issues with the strain induced to the computational elements. For that reason it is used for the simulation of breaking waves, impinging jet, sloshing fluids and generally in the simulations of violent phenomena with very large deformations.

For hydrodynamic applications, we treat the described medium as weakly compressible, so we usually use the weakly compressible SPH method. This method is simple to implement and it can be parallelized efficiently.

Despite their intrinsic capability for simulation of violent free-surface fluid flows, particle methods have a few drawbacks that may considerably affect their accuracy and performance. Such drawbacks are mainly caused by the interpolation features of particle methods; that is, local kernel-based interpolations on the basis of moving calculation points (particles). Non-exact conservation of momentum [2], lack of interpolation completeness [11] and existence of spurious pressure fluctuations are among the major drawbacks associated with particle methods.

In this paper, we first present a short overview of the recent improvement for the treatment of the evaluation of pressure field. Then, we present our improvement of a centered formulation for the pressure gradient term with the introduction of a stabilization term proportional to the pressure difference between two neighbor particles. We present a proof for the stability of this new formulation. Finally we present

some numerical results with comparison to the classical SPH scheme.

## II. RECENT OVERVIEW

There are different ways to improve the pressure calculation in SPH formulations. To avoid the spurious in calculation of pressure field, Monaghan *et al* [9] introduced an artificial viscous term based on a Neumann-Richtmyer artificial viscosity to dampen the oscillations appearing in shock waves. Such an artificial viscosity term also helped to stabilize the SPH scheme and reduce spurious oscillations. Nowadays the most common method for avoid these oscillations are ALE-SPH, density reinitialization and SPH with diffusive term. We quickly present the first two, and we detail the diffusive term method.

### A. ALE-SPH

The SPH-Arbitrary Lagrangian Eulerian (ALE) method, was proposed by Vila [14]. This method relies in the discretization of the inviscid Euler equations, under an ALE description, using SPH approximations. The resulting method resembles more to the finite volume method, using the Godunov method for calculating the fluxes between the volume. The great advantage of the SPH-ALE method is that it enables robust handling of the boundary conditions. Moreover, the Godunov method introduces numerical diffusion, damping in pressure oscillations and provides much smoother results than the standard SPH method.

This method has considerable differences from the traditional SPH. First of all, the conservative system of the Euler equations is solved  $[\rho, \rho u, \rho v, \rho w]$ , instead of using the primitive variable set of the standard SPH method. Also, it adopts an arbitrary Lagrangian Eulerian point of view, meaning that the computational elements move because of the influence of a transport field. Hence the particles may move following the flow field (Lagrangian description), or may remain still (Eulerian description), or move in any other arbitrary way.

# Towards both numerical consistency and conservation for SPH approximation

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**Abstract**—SPH approximation of the gradient of a scalar field involves a calculation of an integral, which is further approximated by the summation over all particles in the support domain. This further approximation step introduces an error and generally leads to the failure of zero-order consistency, that is, SPH approximation does not exactly reproduce a constant field. The usual correction to achieve zero-order consistency is implementing the reproducing approximation kernel. However, such kernel violates one of the most important properties of the SPH method, that is, the full conservation which is assured by the anti-symmetric algorithm for particle-particle interactions.

In this contribution we show that the conditions under which a SPH formulation can satisfy the properties of conservation and zero-order consistency at the same time is the so-called partition condition. This condition can be achieved by relaxing particle under constant pressure field and the resulted particle distribution has the radial distribution function (RDF) very similar to that of water molecules. We also show that, with two different kernel functions, the SPH approximation on particles following the partition condition can achieve very high-order convergence respect to the ratio between the inter-particle space to the radius of kernel support.

## I. INTRODUCTION

Smoothed particle hydrodynamics (SPH) is a mesh-free Lagrangian simulation method introduced by [8] and [4]. It has a wide range of applications ranging from structural mechanics to complex multi-phase flows [10], [11]. In SPH a discretization element is called particle and every particle can take an arbitrary position in space. At a particle position  $\mathbf{r}_a$  the gradient of a scalar field  $\psi(\mathbf{r})$  is approximated by using the following three-step approach:

$$\begin{aligned} \nabla\psi(\mathbf{r}_a) &\approx \int_V \nabla\psi(\mathbf{r})W(\mathbf{r}_a - \mathbf{r}, h) dV \\ &= - \int_V \psi(\mathbf{r})\nabla W(\mathbf{r}_a - \mathbf{r}, h) dV \quad (1) \\ &\approx - \sum_b \psi(\mathbf{r}_b)\nabla W(\mathbf{r}_a - \mathbf{r}_b, h)V_b \end{aligned}$$

where  $W(\mathbf{r}, h)$  is a kernel function which depends only on the magnitude of the vector  $\mathbf{r}$ , and has a compact support domain. The parameter  $h$  is called smoothing length and if it tends to zero  $W(\mathbf{r}, h)$  approaches the Dirac delta function.

The first step in Eq. (1) is called filtering or smoothing approximation and an error introduced by this stage is called

the smoothing error. The second step is an integration by parts and we assume that the kernel function is zero at the edge of support domain. The third step calculates integral by the summation over all particles in the support domain, and  $V_b$  denotes the volume of the particle  $b$ . We call the error of the last stage the integration error.

The quality of the SPH method is directly determined by the properties of the above two approximation errors. And it is not surprising that equation (1) was studied extensively. Monaghan [10] showed that for sufficiently smooth kernel the smoothing error is  $O(h^2)$ . Quinlan et. al. [12] analyzed the integration error analytically for uniformly spaced particles and numerically when these particles are randomly perturbed. It is found that, while for uniformly spaced particles high-order integration error is obtained, for the later case the integration error lacks the zero-order consistency, in other words the equation (1) does not exactly estimate the zero derivative of a constant-valued function, which is known as a major difficulty of SPH. And several modifications of the method were proposed to remedy this problem such as the reproducing kernel particle method (RKPM) [7]. However, as will shown later, such kernel violates the conservation property, which is one of the most important properties of the SPH method.

In this paper we begin with the simple integration rule, that is, a zero-order consistency of derivative estimate can be achieved in equation (1) when the sub-domains defined by the particles give a partition of the entire domain. Furthermore, inspired by our previous work [1], we show that this condition, without compensating the property of discrete conservation, can be achieved by relaxing particles under constants pressure, and also demonstrate by numerical experiments that the convergence rate of the integration error is close to that for uniformly spaced particles.

## II. ANTI-SYMMETRIC FORM OF THE SPH APPROXIMATION OF DERIVATIVE

In the literature there are several forms of SPH approximation of derivative. In this section we specify a class of such approximations which is popular in hydrodynamic simulations.

We construct an approximation to the function  $\nabla\psi(\mathbf{r})$  at position of a particle  $a$ . We start by adding an equal-to-zero term and then apply transformation (1) to the both terms. After

# On the model inconsistencies in simulating breaking wave with mesh-based and particle methods

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**Abstract**—In the present work the numerical simulation of breaking wave processes is discussed. A detailed analysis is performed using Smoothing Particle Hydrodynamics (SPH) models as well as a mesh-based Level-Set Finite Volume Method (LS-FVM). Considerations on the numerical dissipation involved in such models are discussed within the frameworks of weakly compressible and incompressible assumptions. The breaking wave processes are simulated using both mono- and two-phases models. Due to the extensive test-cases discussed, the present analysis is limited to a bi-dimensional framework. Test-cases with increasing complexities are considered starting from a simple 1D impact of two water-jet up to complex shallow water breaking waves. The analyses presented in this article are not only useful to weakly compressible SPH or LS-FVM users but can be extended to other numerical models for which accurate (convergent) results on benchmark test-cases are provided

## I. INTRODUCTION

Free surface flows are challenging phenomena to model and simulate due to the possible fragmentation and reconnection of the air-water interface. Starting from the 80s when the volume of fluid technique (VOF) was developed, the numerical simulation of fluid-fluid interactions have been tackled by many researchers (see e.g. [1]). Besides the VOF approaches, in the framework of mesh-based method another free-surface tracking algorithm have become quite popular: the so called Level-Set (LS) method [2]). More recently also the development of particle-methods has allowed to study free-surface complex flows (see e.g. [3]). Indeed, thanks to the meshless and lagrangian characters of such methods it is possible to simulate liquid fragmentation in a natural way. For this reason in the last twenty years hundreds of articles regarding the simulation of free-surface flows through Smoothed Particle Hydrodynamics (SPH) (see e.g. [4]) or Moving Particle Semi-implicit (MPS) solvers (see e.g. [5]) have appeared in the literature.

All the above-mentioned numerical methods can hide model inconsistencies when simulating liquid fragmentation and reconnection (both involved in breaking phenomena). For instance, as demonstrated in [6], in simulations involving liquid collisions, the incompressible assumption implies instantaneous mechanical energy losses. Another important aspect is related to the use of mono-phase or two-phase models for simulating breaking wave events. The mono-phase model give rise to another model inconsistency when cavity collapses

occur since it can lead to a very different flow evolution with respect to the case where air-cushion effects take place (see e.g. [7]). On the other hand, in many two phase model the air phase is considered incompressible and therefore the air-cushion effects can not be taken into account. Notwithstanding these model inconsistencies different articles in the recent literature show that mesh-based and particle solvers are able to solve breaking wave and the related energy dissipation (see e.g. [8], [9], [10]).

This work is devoted to a critical analysis of these and other model inconsistencies and to show the consequence on the numerical results. We focus our attention on the SPH model and on a Level-Set Finite-Volume-Method (LS-FVM). The two solvers selected take advantage of quite different numerical approaches, that is a Lagrangian Particle Methods and a classical mesh-based method; therefore, the conclusions we draw can be of interest also for other kinds of numerical solvers. Furthermore, in the SPH model here adopted the liquid is treated as a weakly compressible media while in the LS-FVM an incompressible constraint is used. This allow us also to consider these two different models when dealing with water impacts and/or breaking waves.

After a brief introduction of the governing equations and the SPH and LS-FVM models, we start our analysis on the simple problem of two impinging jets in 1D which allows the discussion of the energy transfer features of the different models. Then, the problem of 2D impinging jets is discussed as prototype problem useful to address cavity collapse during breaking event. The role of the free-surface and the different behavior on the energy conservation of the solvers is discussed. Finally, a confined dam-break flow is considered. Indeed, this problems is characterized by different stages: (i) an inviscid fluid deformation, (ii) a water impact on a vertical wall, (iii) a backward plunging jet formation, (iv) splashing stage with several cycles (v) finally a sloshing flow regime. Because of these stages it is possible to consider different energy dissipation processes. This final problem is studied using a single-phase model as well as a two-phase model showing how the two different models adopted behave in simulating such a flow.

# Modeling the coherent vortices in breaking waves

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**Abstract**—Breaking water waves at the shoreline create a wide range of turbulent structures in the water column. Plunging waves are particularly interesting as the plunging tip of the wave impacts into the toe of the wave, often creating a tube or barrel of air that surfers enjoy. As a result, the turbulence left after the passage of the wave consists, in part, of coherent horseshoe (hairpin) vortices that sink deeper into the water column with time. Nadaoka et al. (1989) identified the legs of the horseshoe (hairpin) vortices as obliquely descending eddies; here we show they are just part of the horseshoes (hairpins). We also provide an argument for the creation of these hairpin vortices (Farahani et al., 2014b), based on an analogy with turbulent boundary layers.

## I. INTRODUCTION

Water wave breaking at the shoreline produces turbulence, which can play an important role in the sediment transport, wave damping, and safety of vessels and structures located in the surf zone (Banner and Peregrine, 1993). Not only do waves periodically breaking on a beach give rise to these coherent vortical structures, but a solitary wave does as well. One of the important differences with a solitary wave (which is a first order approximation of a tsunami) is that here there is no pre-existing turbulence in the water column prior to the arrival of the wave as is the case for waves on beaches. Therefore, we can study three-dimensional vortex structures separately from the effect of returning undertow and the residual turbulence induced from the previously broken waves in the case of periodic waves.

Breaking water waves including solitary waves have been previously modeled using Smoothed Particle Hydrodynamics (SPH) method by several researchers such as Monaghan and Kos (1999); Monaghan and Kos (2000); Dalrymple et al. (2002); Colagrossi and Landrini (2003); and Dalrymple and Rogers (2006). In this study, we use three-dimensional Smoothed SPH method to model broken solitary waves as well as to investigate the induced three-dimensional vortex structures and turbulent fields. Two different solitary wave types (spilling wave and plunging wave) are studied and coherent vortex structures associated with each type are investigated. Our computations are carried out with the GPUSPH model

(Hérault et al. 2010), which uses massively parallel Nvidia graphics cards.

## II. GOVERNING EQUATIONS AND GPUSPH MODEL

The governing equations to model the water wave motion consist of the conservation of mass and the conservation of momentum as:

$$\frac{\partial \rho}{\partial t} + \rho(\nabla \cdot \vec{u}) = 0 \quad (1)$$

$$\frac{D\vec{v}}{Dt} = -\frac{1}{\rho}\nabla P + \vec{g} + \vec{\Theta} \quad (2)$$

where  $\rho$  is density;  $t$  is time;  $\vec{u}$  is velocity;  $P$  is the pressure;  $\vec{g}$  is the gravitational acceleration; and  $\vec{\Theta}$  is the viscous term. The conservation of mass equation can be written in SPH form as:

$$\frac{\partial \rho_a}{\partial t} = \sum_b m_b (\vec{u}_a - \vec{u}_b) \nabla_a W(r_{ab}) \quad (3)$$

where  $a$  denotes the particle of interest;  $b$  denotes the neighboring particle;  $m$  is the particle mass;  $W$  is the kernel function; and  $r_{ab}$  is the distance between particle  $a$  and particle  $b$ .

The first term of the right hand side of the momentum equation (2) is the pressure gradient term that can be written in the SPH form as:

$$-\sum_b \left( \frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) m_b \nabla_a W(r_{ab}) \quad (4)$$

The second term on the right hand side of the momentum equation is the gravitational acceleration, which is defined as:  $\vec{g} = (0, 0, 9.81) \frac{m}{s^2}$ . The third term on the right hand side of the momentum equation is the viscous term that can be computed using several methods. In this study we have used the SPS approach of Dalrymple and Rogers (2006) with constant Smagorinsky coefficient. In the SPS approach, the effect of turbulence is considered in the SPH method using a model similar to the Sub-Grid Scale (SGS) turbulence model in the Large Eddy Simulation (LES) method (Dalrymple and Rogers, 2006).



# SPH Numerical computations of wave impact onto a vertical wall

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**Abstract**—In order to assess wave impacts on coastal structures that are coupled with a marine energy device, a SPH software (JOSEPHINE, [1]) is used and new features are developed. The present paper will focus on pressure peaks prediction onto a vertical wall in terms of accuracy and convergence of the used SPH scheme. Firstly, an idealised configuration representing a wave impact (*i.e.* impact of triangular liquid column) will be considered. This test case allows us to investigate the relationship between free surface shape and impact dynamics. The results are compared with those obtained from other numerical VOF (Volume Of Fluid) computations of Mokrani *et al.* [2] using THETIS software and the analytical results of Wu [3]. Secondly, the generation and propagation of a solitary wave is computed in a wave flume equipped with a beach, which makes the solitary wave breaks onto a vertical wall. Several types of impact are obtained similarly to those mentioned in literature by changing the wave-maker parameters or the water depth in numerical wave flume. The results will be compared with experimental data.

## I. INTRODUCTION

This study is performed under the framework of the project EMACOP (Energie MArine COtière et Portuaire) funded by the French Ministry of Ecology, Sustainable Development and Energy. This project focuses on multifunctional structures equipped with a coastal wave energy recovery device. The device that will be assessed during this study is an oscillating water column. The final aim being evaluating its survivability in high or extreme weather conditions, impacts of energetic waves will be considered. This practical problem involves complicated free surface deformations. SPH is an ideal approach to simulate such a process due to its mesh-free, Lagrangian numerical scheme.

The accuracy of computed impact pressure still being a scientific issue (see for instance Mokrani *et al.* [2], [4] or Rafiee *et al.* [5]), an analytical test case will be first considered. The academic test case is basically the hydrodynamic impact due to a triangular water column hitting on a solid wall. By increasing the angle of the triangular water column, more and more violent impacts are obtained. This test case reveals to be complicated in terms of convergence and stability of the numerical method. Our numerical results are compared with the analytical results of Wu [3] for the validation of our SPH model. Finally, this academic case allows us also to assess the stability and accuracy of different SPH approaches, namely the WCSPH method with a Rusanov flux and  $\delta$ -SPH.

Then wave impacts, more similarly to the practical problem mentioned above, are presented in the final section. A numerical wave-maker generates a solitary wave, which propagates in a wave flume and finally starts to break. The impact pressures and forces on the wall are thus presented and analysed.

## II. WEAKLY COMPRESSIBLE SPH MODEL

In our problem, the governing equations are the Euler equations in the Lagrangian frame for a weakly compressible and inviscid fluid. The Tait's equation of state is used to close the system of equations:

$$P_i = \frac{\rho_0 c_0^2}{\gamma} \left( \left( \frac{\rho_i}{\rho_0} \right)^\gamma - 1 \right) \quad (1)$$

where  $\rho_0$  is the density at the free surface,  $\gamma = 7$  is the polytropic characteristic exponent of the fluid and  $c_0$  is the numerical sound speed. Here, the sound speed is set so that  $c_0 = 10|u_{max}|$ . In our model, the smoothing kernel  $\eta_\epsilon^0$  is a truncated Gaussian function proposed by Colagrossi and Landrini [6]. In the sequel, in order to assess the stabilisation properties of different SPH variants, two of them will be tested in section III thanks to an academic test case.

### A. Diffusive terms

Different variants of the diffusive term ( $\mathcal{D}_i$ ) to be added to the continuity equation (eq. (2)) were proposed in the SPH literature.

$$\frac{D\rho_i}{Dt} = -\rho_i \sum_j \mathbf{u}_{ij} \cdot \nabla_i \eta_\epsilon^0(\mathbf{x}_{ij}) \frac{m_j}{\rho_j} + \mathcal{D}_i, \quad (2)$$

In this paper, two different approaches of this diffusion term are presented and tested, namely the Rusanov flux and  $\delta$ -SPH. Both of them can be expressed similarly and as the following:

$$\mathcal{D}_i = \sum_j \psi_{ij} \mathbf{n}_{ij} \cdot \nabla_i \eta_\epsilon^0(\mathbf{x}_{ij}) \frac{m_j}{\rho_j}, \quad (3)$$

with  $\mathbf{x}_{ij} = \mathbf{x}_j - \mathbf{x}_i$ ,  $\mathbf{u}_{ij} = \mathbf{u}_j - \mathbf{u}_i$ ,  $\mathbf{n}_{ij} = \frac{\mathbf{x}_{ij}}{|\mathbf{x}_{ij}|}$ .

For the Rusanov flux, following the work of Ferrari *et al.* [7], the remaining term  $\psi_{ij}$  can be written as:

$$\psi_{ij} = c_{ij}(\rho_j - \rho_i - \Delta\rho_{ij}), \quad (4)$$

# Modelling Of Wave Impacts On Harbour Structures And Objects With SPH And DEM

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**Abstract**—A Smoothed Particle Hydrodynamics (SPH), coupled with a Discrete Element Method (DEM), is presented and applied to model the interaction of incoming waves over a section of a shipping harbour. The main objective is to simulate the response of the containers at a harbour in Portugal to the hydrodynamic action represented by a tsunami wave. Wave amplitude is taken from data of the coast of Portugal and the discretization of the port geometry and infrastructures is based on high resolution digital elevation models and actual port information. Buildings and terrain are treated as fixed boundary, with a series of shipping containers and a large vessel being treated as unrestricted rigid bodies with different material properties (density, Young modulus, Poisson and friction coefficients). In the model, the fluid is modelled with the Navier-Stokes equations, solved by the SPH method. This allows for the simulation of a large spectrum of relevant momentum transfer scales between fluid and solid phases. The solid interactions are accounted for by considering physically based formulations derived from contact mechanics and discretized as a DEM, in what constitutes the main novelty of the proposed work. The GPU implementation of DualSPHysics allows for the high resolution spatial discretization covering the large domain at a reasonable computation time. Experimental and numerical data are used to validate the formulation and to assess the accuracy and limitations of the model, both considering fluid-solid interactions and solid-solid contacts. The behaviour of containers and the carrier vessel is tracked and could offer insights on the potential risk to the integrity of main port infrastructures. A larger simulation would be needed to consider critical structures as they are located mostly inland, requiring Multi-GPU simulations to compensate for the larger domain.

## I. INTRODUCTION

The interaction of solid material in fluid flows is common in several fields, including coastal, offshore, maritime and fluvial engineering. In such contexts, it can be associated large scale disasters that pose a relevant risk to populations and infrastructure. The main difficulties with modelling such class of events arise from the characteristics of the phenomena. The scale of the affected area implies that modelling a single event may require very large domains, since the non-linear nature of the flow difficults the partition of the same in several smaller, individual domains and events. Another type of scale issue arises from the type of interactions, that may require very high resolution to resolve to a proper extent. The type of non-linear and multiscale problem that is being addressed poses severe

limitations to the usage of simple models [1]. Furthermore, experimental validation of such models is remarkably complex and also relies on simplifications, both on the setup and on the analysis of the data [2], [3].

Any computational tool designed to deal with such problems must be computationally scalable and should be able to model all physically relevant scales which fluid-solid interaction occurs. In most engineering applications involving fluids and structures, solid objects are much larger than the smallest flow scales. For instance, viscous modes of momentum transfer are often negligible since the involved Reynolds numbers are normally large [2]. However, the relevant modes of interaction are not always evident, in which case the model must be designed to offer high spatial and temporal resolutions. Also, to minimize the influence of non-physical boundaries, some simulations require remarkably large domains. This stresses the need for high performance models and implementations. Finally, such models should be based on consistent conceptual models, avoiding *ad hoc* closures, and should be subjected to a computational implementation that preserves the key mathematical properties of the conceptual model.

Within the meshless framework, efforts have been made on unifying solid and fluid modelling. Such is appealing since if the fluid phase is well discretized then most of such scales should be represented. Reference [4] modelled a rigid body as a collection of Moving Particle Simulations (MPS) fluid particles, rigidified by default. This has become the standard approach due to its simplicity and good results. Similarly, [5] modelled the effects of wave interaction on a caisson breakwater resorting to Smoothed Particle Hydrodynamics (SPH) and some special considerations for the particles that made up the solid body, effectively including a form of frictional behaviour. For normal interactions the continuum potential based forces of the form used in [5], [6] are not based in mechanics of contact of rigid bodies. Contact laws like the non-linear Hertzian models have been used extensively in the Discrete Element Method (DEM) literature [7], being regarded as one of the most, physically based, available class of contact laws. Further generalization allows for the inclusion and consideration of distinct materials in such interactions [8].

This work describes a model where inter particle forces of

# Hydrodynamic performance simulations using SPH for automotive applications

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**Abstract—** In the automobile industry, CFD is mostly used to improve the aerodynamic performance of cars and not much has been done yet concerning hydrodynamic flows. Problems like the tire aquaplaning or ford crossing remain difficult to be simulated using traditional meshed based methods, e.g. Finite Volume method. In these flow problems, the free-surface is very complex (with a lot of discontinuities) and the flow is very violent, not to mention the fact that complex geometries are treated and that the relative motion between the car and the tires is to be considered. All these aspects combined make it difficult for any meshed based method to simulate efficiently these flows. In this article we will present a series of results showing that with SPH, it is possible to achieve both global and local convergence for such complex flows. Focus is also given to the analysis of these problems by changing some parameters as the tire speed and the water layer depth for the aquaplaning problem. In the figure below we show the free-surface shape for the tire aquaplaning simulation using 5 million particles and for a ford crossing simulation using 24.5 million particles. These simulations were performed using the SPH-flow code with the Riemann-SPH formulation and up to 1 billion particles.

## I. INTRODUCTION

In the automobile industry much effort is concentrated into performing CFD computations of the aerodynamic performance of cars. Several examples may be found in literature concerning Formula 1 simulations. However, in the specific case of hydrodynamic simulation not much can be found in such a field. Indeed, considering the external flows, the air flow around the vehicle is the phenomenon that impacts the most its energy efficiency. However other phenomena like tire aquaplaning, ford crossing and windshield wiping are also important and must be considered.

Due to the complexity of the geometry of the car and its appendices (e.g. tire shape in Figure 1), the modelling of the flow around such complex structures can become very complicated with mesh based methods. Very fine meshes may be necessary, not to mention the fact that meshing complex geometries can sometimes be time-consuming and impact the quality of results. In [12], we may find results for the tire-aquaplaning using a mesh-based method.

For the past years the SPH algorithm has been proven to be a very robust method to handle complex flows around complex geometries as one can see in [1-6] (limited list of articles). The SPH method seems, then, to be well suited to model such complex hydrodynamic flow phenomena taking place in the automobile industry. The Smoothed Particle Hydrodynamics algorithm handles easily with discontinuities in the flow (it intrinsically takes into account their presence)

and the user does not need to worry with the mesh generating process: the particles distribution can be straightforwardly adapted to any kind geometry, even as those present in the automobile industry.

Moreover, the external flow phenomena like tire aquaplaning can be extremely violent if one considers elevated speeds and very complex with several discontinuities in the flow: it is split by the stripes.



Figure 1 – Tire geometry with its complex stripes

In this article we will present a series of results for these automobile applications demonstrating how suitable SPH can be to simulate such flows phenomena. Focus will be given to the tire aquaplaning flow and to the ford crossing.

Additionally, in this article it will also be demonstrated that with SPH one can achieve local and global convergence. Taking as example the tire aquaplaning, we can demonstrate convergence on global loads on the tire but also we can seek convergence looking at pressure probes inside the tire stripes. Considering that the tire stripes may measure some millimetres, convergence can be hard to be achieved and maybe only achieved by using a high number of particles. The results shown in this article regarding this aspect may be of the interest of the research community.

The present article is subdivided as follows: first a section introducing the SPH algorithm used is presented followed by the presentation of the description and results of the tyre aquaplaning and the ford-crossing test cases respectively. Conclusions close the article.

## II. SPH ALGORITHM

The results presented in this article were achieved using the SPH-flow code developed by HydrOcean and Ecole Centrale de Nantes. The SPH-flow code has all the main variants of the SPH method together with the most recent developments in the area:

# Simulation of earthquake sloshing loads in a nuclear reactor

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**Abstract**—Modelling of sloshing flow inside a Lead-cooled Fast Nuclear Reactor during an earthquake is conducted, focusing on the evaluation of the loads caused by the fluid on the structure. AQUAgpusph, a free software OpenCL accelerated SPH code has been used. This tool is analysed, including the performance comparison with some available GPU accelerated SPH codes, and its validation against SPHERIC test case number 10 about severe sloshing phenomena. SPH fits particularly well to this application due to the complex nuclear reactor geometry. Simulations have been conducted with ELSY lead-cooled fast reactor geometry.

## I. MOTIVATION

In the design process of nuclear reactors, the loads during an earthquake due to the sloshing phenomena have been considered in the past using semi-empirical techniques [18]. However after the violent earthquakes in Japan which caused the collapse of nuclear plants (Kashiwazaki-Kariwa in 2007 and Fukushima in 2011), the nuclear engineering community has significantly increased the research efforts on this topic [16]. More specifically, the fluid-structure interaction is becoming one of the points which is attracting the attention of the researchers [9].

In this sense, due to the complex geometries considered in these problems where mesh based methods may be hard to be applied, the meshless methods are gaining relevance. Particularly SPH has demonstrated to fit well to problems with a complex geometry or heavy free surface fragmentation. However, the characteristic pressure noise shown in the Weakly Compressible SPH (hereinafter WCSPH) formulation may be an impediment to apply this methodology to the fluid loads prediction.

In this paper the simulation of a Lead-cooled Fast Nuclear Reactor (Hereinafter LFR) during an earthquake to evaluate the loads caused by the fluid on the structure is described. We focus on the time spent per simulation and the quality of the measured pressure. The simulations have been carried out with AQUAgpusph, an OpenCL accelerated SPH code [8].

This paper is organized as follows: First, the AQUAgpusph performance is analysed, comparing it with other SPH codes accelerated with CUDA [14, 17]. Second, the results of a simulation of the benchmark test case number 10 are discussed in order to validate the tool [13, 21, 22, 7]. Third,

the nuclear reactor geometry and the earthquake motion is described. Fourth, the results obtained for the Lead-cooled Fast Nuclear Reactor are presented. Finally, a conclusions summary together with future work targets are provided.

## II. PERFORMANCE ANALYSIS

### A. General

In the first stages of a nuclear reactor design process a lot of earthquake potentially critical situations must be simulated to estimate the loads suffered by the structure. More specifically the cases matrix may include a wide variety of combinations of earthquake induced motions and dampers. Hence the performance of the simulation tool is a critical point which must be taken into account. Actually with the classic mesh based models time lapses of order of months per simulation are required to get quality enough results, which are unacceptable [6].

On the other hand, GPU based acceleration technologies have demonstrated to fit pretty well to the SPH codes, at least in the WCSPH formulation, where no linear systems resolution is required, such that a medium size cluster computational power can be achieved by a fraction of its cost [14, 17]. However, almost fully GPU accelerated SPH alternatives have been written in CUDA language, with the intrinsic limitation to NVidia computational devices. Therefore, the AQUAgpusph performance, which is accelerated with OpenCL [8], must be analysed in order to demonstrate that it is competitive in computational terms.

To do that a dam break case is simulated. The dam break problem has been widely used to analyse the performance of CFD codes [23, 19, 5].

### B. Case description

In this work the experiments carried out by Lobovský et al. [20] will be considered, and more specifically the water level  $H = 0.3$  mm case. In Fig. 1 an schematic view of the experimental setup is depicted. An initial column of fluid in rest state, subjected to hydrostatic pressure, evolves freely up to 1.25 seconds. The water level is recorded along the simulation in the positions H1, H2, H3 and H4, as well as the pressure at the solid vertical wall downstream the dam in the

# Modelling real-life flows in hydraulic waterworks with GPUSPH

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**Abstract**—We simulate two real-life cases, a vertical-slot fish-pass and a dam-break with floating objects, using GPUSPH, an implementation of the SPH method in CUDA which has been recently extended including support for fully coupled fluid/solid interaction with moving rigid bodies. Boundary conditions are computed using the unified semi-analytical model proposed by Ferrand *et al.* and include the treatment of turbulence through the Reynolds-averaged  $k$ - $\varepsilon$  model. SPH is also used to compute the total force and torque acting on the floating objects, which are then used to integrate the motion of the objects.

## I. INTRODUCTION

Applications of SPH to real-world problems depends on the correct evaluation of boundary forces, particularly when the domain has a complex shape and to model fluid/object interactions accurately. We show the use of the unified semi-analytical boundary model proposed by Ferrand *et al.* [7] in two problems derived from real-world scenario: a vertical slot fish-pass and a dam-break with floating objects on a natural topography.

The simulations are done with GPUSPH [5], an implementation of 3-D SPH using CUDA-enabled GPUs to achieve high computing performance. GPUSPH has been recently extended to include the unified semi-analytical boundary model, and support for floating objects and their fully coupled interactions with the fluid. The domain boundaries are described as a triangular mesh (stored in STL format) which is pre-processed by Crixus, a tool that computes the initial values for the boundary correction terms (see section II-A) and can provide fluid particle distributions to fill domains with arbitrary shapes. Crixus' output can then be imported into GPUSPH to run the actual simulation. Floating objects are discretized as thin shells of boundary particles, whose interaction with the fluid is used to compute the total force and torque acting on the object. GPUSPH then relies on the open-source ODE library to integrate the object motion and to compute object/object interactions as well as the interaction of the objects with the topography.

We will first briefly summarize the key aspect of the unified semi-analytical boundaries and of the  $k$ - $\varepsilon$  turbulent viscosity

models we use in our applications (section II), followed by the results of their application to a vertical-slot fish-pass (section III). This is followed by a synthetic description of our approach to the modeling of fluid/solid interaction, an additional theoretical aspect underlying the simulation of a dam-break with floating objects (debris flow on a spillway, (section V). Conclusions are then drawn in section VI.

## II. UNIFIED SEMI-ANALYTICAL BOUNDARY CONDITIONS AND SPH $k$ - $\varepsilon$ TURBULENT VISCOSITY MODEL

In our presentation of the semi-analytical boundary model, we will use the standard notations for weakly-compressible SPH (WCSPH), where  $W$  denotes the smoothing kernel with influence radius  $h$ ,  $\Delta p$  is the average inter-particle distance,  $\mathbf{r}_a$  the position of particle  $a$ ,  $\mathbf{r}_{ab} = \mathbf{r}_b - \mathbf{r}_a$  denotes the distance vector between the particles,  $r_{ab}$  its norm and  $W_{ab} = W(r_{ab}, h)$ . For the physical properties we will use the usual subscripted convention, with  $\rho_a$  being the density of particle  $a$ ,  $m_a$  its mass,  $V_a$  its volume,  $P_a$  its pressure and  $\mathbf{u}_a$  its velocity. Additionally we will denote by  $\mathcal{F}$  the set of all fluid particles, and by  $\mathcal{S}$  the set of all boundary particles.

The flow is assumed weakly compressible with an equation of state (EOS)  $P = B((\rho/\rho_0)^\zeta + 1)$  where  $\zeta = 7$  is the polytropic constant,  $\rho_0$  the at-rest density of the fluid and  $B = \rho_0 c_0^2 / \zeta$ ,  $c_0$  being the numerical speed of sound density of the fluid.

### A. Renormalization terms

The unified semi-analytical boundary model was first introduced by Kulasegaram *et al.* [3], suggesting a renormalization for the SPH smoothing kernel near a solid wall. In such a case, the standard WCSPH density summation  $\rho_a \simeq \sum_{b \in \mathcal{F}} m_b W_{ab}$  is replaced by

$$\rho_a = \frac{1}{\gamma_a} \sum_{b \in \mathcal{F}} m_b W_{ab}.$$

The renormalization factor  $\gamma$  is defined as

$$\gamma_a \equiv \int_{\Omega \cap \Omega_a} W(|\mathbf{r} - \mathbf{r}_a|) dV$$

# Application of GPUSPH to Design of Wave Energy

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*Abstract*—Analysis, design and evaluation of wave energy converters involves hydrodynamic which are often nonlinear and not always well handled by linear solutions and somewhat complicated, articulated bodies. This study is about the develop and application of a new approach using Smooth Particle Hydrodynamics (SPH). SPH is a Lagrangian meshless numerical method with substantial capabilities in simulation of both fluid dynamics and solid mechanics due to its meshless nature. GPUSPH is an implementation of SPH on NVIDIA CUDA-enabled (graphics) cards. GPUSPH is used as a simulation tool for both the WET-NZ and the SURGE-WEC wave energy converters in this study

## I. INTRODUCTION

There are many different categories of WECs (Wave Energy Converters) including point absorbers, oscillating water columns, and surge devices. Within each category there are many differently designed devices that are currently being developed and installed most of which are proprietary. Wave energy converters (WECs) are expected to operate and survive in a very hostile environment. Of primary importance is the ability to be designed and constructed to efficiently provide wave energy. Of equal importance is the safety of the device during extreme events whether operating or powered down. Efficient optimization of WEC design beyond the

proof of concept can be initially undertaken with coarse numerical models. Then, confirmation with physical models follows with the numerical modeling continuing at a finer resolution. There are several options available to do the former analysis but very few are able to accurately capture both the hydrodynamics and the structure response especially with articulated structures. WAMIT (Ferreria and Newman, 2008) for example is based upon 1st and 2nd Order potential theory that limits wave breaking and most wave nonlinearities.

Le-Ngoc et al. (2010) discussed the different approaches to modeling a complex hydrodynamic environment with multiple solid objects interacting and the feedback from a power take off system. The direction they chose is to simplify the system to the point where all components can be incorporated into a single MATLAB program.

The objective of this paper is to illustrate the effectiveness of GPUSPH to provide the accurate hydrodynamics needed including the fully nonlinear features of breaking waves and the wave structure interaction. This will be illustrated with the analysis of the laboratory and field-tested WET-NZ by Pacific Energy Ventures and with the SurgeWec developed by Resolute Marine Energy.

# Multiphase and free-surface flows in the finite volume particle method

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**Abstract**—The finite volume particle method (FVPM) has been developed to enhance its modelling capability for free-surface and multiphase flow. Results are presented for benchmark applications of various hydrostatic cases, a falling wedge entering water, dambreak flow, and Rayleigh-Taylor instability. The preliminary results presented in this paper confirm that FVPM is a viable tool for free-surface and multiphase flow applications.

## I. INTRODUCTION

The finite volume particle method (FVPM) is a meshless method that resembles SPH in its use of overlapping particles and kernels to discretise the continuum. Unlike SPH, FVPM is built on a weak formulation of the governing equations. It is closely related to the classical finite volume method, and inherits some of its convergence and conservation properties. FVPM has been demonstrated and evaluated for various applications including internal flows, and flow over moving walls and rigid bodies. However, while great progress has been made with SPH in simulation of free-surface and multiphase flows, FVPM has had very limited application in these fields. The purpose of the present work is to adapt FVPM where necessary for the physics of free-surface and multiphase flow, and evaluate it critically in some benchmark applications.

## II. THE FINITE VOLUME PARTICLE METHOD

FVPM is described here in outline. Detailed derivations and analysis of the general FVPM are given by Keck and Hietel [1] and Junk [2]. The implementation used in this work follows Nestor *et al.* [3] and Quinlan *et al.* [4], except where otherwise stated.

The governing equations to be solved are of the form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = 0, \quad (1)$$

where  $\mathbf{U}$  is the vector of conserved variables and  $\mathbf{F}$  is the flux function. To derive the FVPM, the system (1) is multiplied by a test function  $\psi_i(\mathbf{x}, t)$  which is non-zero only in the support of particle  $i$ . The test function  $\psi_i(\mathbf{x}, t)$  is constructed as

$$\psi_i(\mathbf{x}, t) = \frac{W_i(\mathbf{x}(t))}{\sum_j W_j(\mathbf{x}(t))}, \quad (2)$$

where the particle weight function  $W_i(\mathbf{x}, t)$  is compactly supported on  $\Omega_i$ . Each particle moves with an arbitrary transport

velocity  $\dot{\mathbf{x}}_i$ . Application of the test function results in the following semi-discrete form of the FVPM:

$$\frac{d}{dt} \int_{\Omega} \psi_i(\mathbf{x}, t) \mathbf{U} d\mathbf{x} + \sum_j \beta_{ij} \mathcal{G}(\mathbf{U}_i, \mathbf{U}_j, \dot{\mathbf{x}}_i, \dot{\mathbf{x}}_j) + \beta_i^b \mathcal{G}_i^b = 0. \quad (3)$$

The numerical flux function  $\mathcal{G}$  approximates the flux  $\mathbf{F}$ , as in the classical finite volume method (FVM), and also accounts for transport between particles  $i$  and  $j$  due to relative motion. The superscript  $b$  denotes boundary terms. The vectors  $\beta_{ij}$  and  $\beta_i^b$  take the place of cell-cell and cell-boundary interface areas, respectively, in mesh-based FVM.

Interparticle area  $\beta_{ij}$  is defined as  $\gamma_{ij} - \gamma_{ji}$ , where

$$\gamma_{ij} = \int_{\Omega} \frac{W_i(\mathbf{x}) \nabla W_j(\mathbf{x})}{(\sum_k W_k(\mathbf{x}))^2} d\mathbf{x}. \quad (4)$$

But this definition, interparticle area satisfies  $\sum_j \beta_{ij} = 0$ , which is analogous to the geometric condition that faces of a finite volume mesh cell form a closed polyhedron, and  $\beta_{ij} = -\beta_{ji}$ , which ensures conservative exchanges between neighbours. With the substitution of  $\beta_{ij}$  for cell face area, FVPM can be analysed rigorously as a generalised FVM with cells allowed to overlap [2].

Usually,  $\beta_{ij}$  has been calculated by Gaussian quadrature, which dominates the computational time of the method. Alternatively, if  $W_i(\mathbf{x})$  is defined as 1 inside the support of particle  $i$  and 0 elsewhere, the integrals of 4 are greatly simplified and can be computed analytically. The resulting scheme is both faster and more accurate than FVPM based on quadrature [4].

Particle volume is defined as

$$V_i(t) = \int_{\Omega} \psi_i(\mathbf{x}, t) d\mathbf{x}. \quad (5)$$

This equation is used in practice to initialise and periodically reset particle volume. Differentiation of (5) with respect to time yields

$$\frac{dV_i(t)}{dt} = \sum_j (\gamma_{ij} \cdot \dot{\mathbf{x}}_i - \gamma_{ji} \cdot \dot{\mathbf{x}}_j), \quad (6)$$

which is less costly than (5) and is used to update volume on most time steps.

To evaluate the numerical flux  $\mathcal{G}$ , data is reconstructed to particle interfaces using a linear MUSCL procedure [5] with

# Finite Volume Particle Method for 3-D Elasto-Plastic Solid Simulation

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**Abstract**—Finite Volume Particle Method was successfully used to predict fluid flow behavior for 2-D simulations. In this paper, we present a FVPM which is applicable for 3-D solid mechanics simulations. This method features rectangular top-hat kernels for computing the interaction vectors exactly and efficiently. We employed this method to solve the elasto-plastic constitutive equations. To validate the model, we study the impact of rigid spherical particle to the solid surface with different velocities and compare the residual stress and plastic deformation with the FEM solutions.

## I. INTRODUCTION

Fluid flow advecting silts originating from snow, glaciers or monsoons can cause severe erosion when passing through the turbines. Erosive wear occurs when silt particles collide into the material and remove part of it due to the repeated plastic deformations. The purpose of this paper is to present a particle-based method, which is capable to predict the plastic behavior of the material under the silt impact loads.

The Finite Volume Particle Method (FVPM) is a particle-based method introduced by Hietel [1]. This method includes many of the desirable features of mesh-based finite volume methods. FVPM profits from particle interaction vectors to weight conservative fluxes exchanged between particles. In this methods, computational nodes are usually moving with material velocity which is compatible with the Lagrangian form of the motion equations. FVPM has some features of SPH but unlike SPH, it is locally conservative regardless of any variation in particle smoothing length. This enables the users to refine the solution by splitting particles into smaller ones in the region of interest and perform the simulation efficiently. Recently, Quinlan and Nestor [2] proposed a method to compute the interaction vectors for 2-D cases exactly. Following their work, Jahanbakhsh [3] developed an exact FVPM applicable for 3-D cases. This method features the rectangular top-hat kernel and is implemented in SPHEROS software [4].

In the present paper, we discretize the elasto-plastic constitutive equations based on the mentioned 3-D FVPM. To validate the model, we select a problem concerning the shot impact to the solid material. This test case is selected due to its close relation to erosive wear mechanism. The numerical study is performed for normal impact of a single shot to the solid plate. We study the effect of two impact velocities of

75 and 100 m s<sup>-1</sup>. We validate the method by comparing the residual stress and plastic deformation with the FEM solutions of Meguid et al. [5] and Hong et al. [6].

The structure of the paper is as following. In the next section, we present the governing equations including constitutive model for solid, silt motion and the contact force. Then, FVPM with rectangular top-hat kernel discretization is presented. Later, the strategy used for particle splitting is explained. We present the solution algorithm and numerical results afterward.

## II. GOVERNING EQUATIONS

### A. Solid state

The solid motion is governed by mass and linear momentum conservation equations as

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{C} \quad (1)$$

$$\frac{d(\rho \mathbf{C})}{dt} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}_c + \rho \mathbf{g} \quad (2)$$

where  $\frac{d}{dt}$  denotes substantial derivative,  $\rho$  is the density,  $\mathbf{C}$  is the velocity vector,  $\mathbf{g}$  is the gravitational acceleration and  $\boldsymbol{\sigma}$  is the Cauchy's stress tensor. To model the effect of silt, the contact force,  $\mathbf{f}_c$ , exerted by silt particles in considered in linear momentum equation.

The Cauchy's stress tensor,  $\boldsymbol{\sigma}$ , is decomposed as

$$\boldsymbol{\sigma} = \mathbf{s} - p \mathbf{I} \quad (3)$$

where  $\mathbf{s}$  represents the deviatoric stress tensor and  $p$  represents the pressure obtained from equation of state

$$p = a^2 (\rho - \rho_o) \quad (4)$$

In (4),  $a$  and  $\rho_o$  denote to the sound speed and reference density respectively. For a given bulk modulus,  $K$ , the sound speed is computed as

$$a = \sqrt{\frac{K}{\rho}} \quad (5)$$

The rate of deviatoric stress,  $\dot{\mathbf{s}}$ , is described by the Jaumann rate of stress,  $\mathbf{s}^\nabla$ , as

$$\mathbf{s}^\nabla = \dot{\mathbf{s}} - \mathbf{s} \cdot \boldsymbol{\Omega} - \boldsymbol{\Omega} \cdot \mathbf{s} \quad (6)$$



# Applications and improvements of the particle finite element method to free surface flows.

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**Abstract**—In this work a new generation of the particle method known as Particle Finite Element Method (PFEM), which combines convective particle movement and fixed mesh resolution, is applied to free surface flows. This methodology, named PFEM-2, presents basically two novel steps: first, the possibility of using larger time steps compared to other similar numerical tools, showing that shorter computational times can be achieved while the solution accuracy is maintained. Second, different improved versions of discontinuous and continuous enriched basis functions for the pressure field have been also developed in order to reconstruct the free surface without artificial diffusion or undesired numerical effects. Combining these two improvements, a variety of free surface flows have been solved in 2D and 3D cases, where the evident advantages of the improvements are remarked. The results of the different free-surface problems solved which include: Rayleigh-Taylor instability, sloshing problems, viscous standing waves and the dam break problem are compared to well validated numerical alternatives and experimental measurements obtaining good approximations for such complex flows.

## I. INTRODUCTION

Hybrid methods are everyday more present in computational fluid mechanics, where the Lagrangian framework given by a particle method is combined with a Eulerian methodology. In these hybrid methods, a fixed or reconstructed every  $k$  time steps grid support part of the pressure and velocity calculation. The original idea, given by Monaghan [3] or later works applied to fluid mechanics [13] where a pure Lagrangian perspective was used during the whole meshless computation, has been in some cases completed using other well known discretization methods as FVM [14] or FEM [7]. The first combination of Lagrangian methods and FEM methods, known as MFEM [9], where an extended Delaunay Tessellation is used to reconstruct the mesh while the fluid evolves.

The next step in this evolution was the first version of the PFEM method [10], which was a robust method designed to solve fluid-structure interaction problems including free-surface, breaking waves, flow separations, etc... where lagrangian particles and meshing processes are alternated with the advantage of having a FEM structure that supports the differential equation solvers. An interesting difference between the PFEM and other particle methods as SPH or MPM [17] is that while latter methods transport mass and consequently

have a volume, PFEM uses non-material points that transport fixed intensive properties of the fluid.

A new strategy known as X-IVAS (eXplicit Integration following the Velocity and Acceleration Streamlines) was developed [6]. This methodology of integrating of convection of fluid particles is based on following the streamlines of the flow in the current time step instead of the particle trajectories, which is a better way to solve the non-linearities of the equations of the flow. Adding this strategy to the original PFEM method, a new methodology called Particle Finite Element Method Second Generation (PFEM-2) [8] appears. The X-IVAS strategy gives the possibility of solving complex flows with large time steps ( $CFL > 1$ ), as well as the presence of the mesh allows accurate solutions of the fractional step method.

The current *Fixed Mesh*-PFEM-2, projects states from particles to nodes preserving the initial background mesh, avoiding remeshing at each time-step. In this approach, mesh nodes and moving particles interchange information through different interpolation algorithms. A detailed explanation of this algorithm is given in Section II.

In this work the PFEM-2 has been used to solve free-surface flows in different problems starting from classical benchmark problems as the Rayleigh-Taylor instability and finishing with problems of industrial interest. To the authors knowledge, this paper presents the first application to free-surface flows where PFEM-2 advantage of using larger time steps compared to other methods is exploited. This analysis includes very accurately demanding problems as those involving two different fluids with high density ratios. Taking into account that the computational time per time-step is similar as the one required by other methodologies, the possibility of increasing the time-step implies shorter global computational times.

The treatment of the free-surface has been done simulating both fluids that share the interface and using a scalar function to identify each fluid. The computation of the free-surface at different positions has been compared to other well reputed Eulerian codes obtaining accurate and numerically stable results but using larger time steps. A wide version of free-surface flows has been studied including a wide range of Froude number situations.

# Voronoi-SPH: on the analysis of a hybrid Finite Volumes - Smoothed Particle Hydrodynamics method

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**Abstract**—The recent articles on the Smoothed Particle Hydrodynamics method show that the method has reached a certain maturity. Researchers have now a better understanding of the method, its limitations and its capabilities. SPH is very suitable to treat violent free-surface flows due to its simplicity when taking into account the presence of the free-surface boundary conditions and flexibility to model complex free-surfaces. Nevertheless, its operators lack of accuracy and for that reason, to simulate some kind of flow phenomena with SPH may become a hard (and sometimes impossible) task. Aiming at increasing the accuracy and the range of applicability of the SPH method, some researchers started developing new techniques to couple SPH to other more precise numerical methods. In this article we will consider the coupling of SPH to a Voronoi-based Finite Volume technique, both based on the solution of the Riemann problem. The goal of this article is to show that such a coupling is possible and that much can be learnt from it. We will present both techniques (SPH and Voronoi-based FVM), discuss the coupling and some problems related to it and then ‘validate’ such coupling on free-surface flows.

## I. INTRODUCTION

The Smoothed Particle Hydrodynamics method has shown, for the past years, to be very robust and applicable to a large variety of flow phenomena. In the recent years, SPH has reached a certain maturity and hence relevant improvements are more difficult to be developed. Yet, several major and relevant improvements were proposed which enhanced some aspects of the method. However, these developments do not change the main drawback of the method which relies on the fact that SPH has imprecise operators. Because of that, the same issues encountered for the classical SPH formulation are always present, that is, the incapability of increasing significantly the time-step, the lack of convergence of operators, the well-known tensile instability issues, etc.

The SPH discrete operators have a limited convergence rate and in a way to restore  $0^{th}$  and  $1^{st}$  order convergence, corrections must be used, (Shepard and renormalization for example [8], [18], [19]). However, these corrections are limited and sometimes produce undesired effects in the flow. We may also cite works done by Colagrossi *et al.* [4] and Marrone *et al.* [15] going in the direction of improving SPH interpolators. However, this solution does not rectify the fact

that SPH operators lack of convergence. In order to improve the order of convergence of SPH operators, a deep change in its structure must be proposed and studied since no simple corrections proved to be both efficient and versatile in all situations. However, that would imply to work on a different method, which shall not result on losing the most interesting property of the method, i.e., the fact that it intrinsically takes into consideration the presence of the free-surface.

Taking as basis the similarity of the SPH discrete operators to the Finite Volume method ones, and considering the recent developments on Voronoi-based Lagrangian FVM [22], this article treats of a new method that couples a Lagrangian FVM to SPH: Voronoi-SPH. The objective of such a coupling is to benefit of the advantages of the Finite Volume method (notably its precision) and the Smoothed Particle Hydrodynamics method (notably the fact that the free-surface conditions are intrinsically taken into account by its operators, which is a hard task in FVM). Hence, we propose a method in which the fluid domain is divided into two zones, one being treated by a Voronoi-based Lagrangian FVM formalism and the another zone where the SPH one is used.

We may add to these objectives the desire of better understanding the SPH method itself. Within this method, even though the volume changes in time, it is not explicitly accessible (from the meshless assumption) and researchers have always been concerned by knowing how it evolves and changes during a simulation. The fact of having a mesh (from the Voronoi tessellation) will (maybe) allow us (and SPH practitioners) to have a better view of volume evolution within SPH. Also, we may say that SPH is known for performing well for some kind of flow phenomena, violent flows of small time duration for example. However, when SPH is applied to slow flow phenomena of long time duration (wave propagation for example) it quickly shows its limitations: CPU costs becomes prohibitive and dissipation becomes too important.

It is necessary to state that in this article the main objective is to demonstrate a “proof of concept”, i.e., we want to take the first steps (and justify them) towards a more precise Smoothed Particle Hydrodynamics algorithm which can also be seen as a more flexible Finite Volume method. This article is

# SPH modelling of wave pressures at vertical and perforated breakwaters

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**Abstract**—This paper deals with the development of a 2D weakly-compressible SPH model to simulate the wave pressures acting on vertical and slotted coastal structures. Particular attention is devoted to investigate the diffusive term in the continuity equation in order to smooth out the high-frequency numerical noise in the pressure field. A hybrid formulation based on the diffusive models of Molteni and Colagrossi [1] and Antuono et al. [2] is proposed. The dynamic pressures acting on the body profile of the breakwaters are evaluated with an interpolating kernel, corrected with Moving Least Squares technique, over the neighboring fluid particles, for every point located at a distance equal to the adopted spatial resolution. The interaction between regular wave trains with vertical and perforated breakwaters are analyzed in time, space and frequency domain. The numerical results are compared with laboratory experiments and other diffusive SPH formulations, varying the magnitude of the adopted diffusive term. On the basis of a root mean square error analysis, the results show that the hybrid formulation gives a better agreement with the experimental data for the majority of the investigated test cases. Moreover, SPH simulations highlight non-linear trends of dynamic pressures in correspondence to geometrical singularities, such as the holes of slotted walls, due to strong pressure drops induced by the loss of wave energy.

## I. INTRODUCTION

Vertical and perforated-wall caisson breakwaters are maritime structures widely used in harbors. The main purpose of the perforated ones is to minimize the wave reflection to guarantee safe navigation during sea storms. The performances of perforated breakwaters are usually analyzed by a structural and a hydraulic point of view [3]. In particular, pressure distributions for vertical and perforated breakwaters have been mainly assessed using empirical and approximated formulas (see e.g. [4] [5]), while the use of advanced numerical tools has been rarely adopted to support their design.

For the optimization of these coastal structures, the correct evaluation of the flow impacts on the structure is fundamental. In this context, the use of standard weakly-compressible SPH models leads to the generation of high-frequency numerical noise in the pressure field that can compromise the numerical solution. Some authors have recently introduced a diffusive term in the continuity equation to smooth out the numerical noise occurring in the pressure field [1] [2] [6] [7]. Even if the formulations of Molteni and Colagrossi [1], Ferrari et al. [6] and Groenenboom and Cartwright [7] show an appropriate smoothing level of spurious high-frequency pressures along solid bodies, they produce a decay of potential energy for a

long simulation time [8]. Conversely, the diffusive model of Antuono et al. [2] is able to preserve the hydrostatic pressure component but it has some limitations in evaluating the dynamic pressures when a flow impacts on a solid boundary.

In the case of a breakwater subjected to wave trains, the flow field is firstly characterized by a slow motion induced by non-breaking waves along the flume (from the wavemaker to the breakwater) and, successively, by a faster motion due to the wave impact in which the magnitude of the pressure peaks is dependent on the type of incoming wave attack [5]. In order to obtain an improved model for the interaction between waves and breakwater walls involving different flow dynamics, a hybrid formulation of the models by Molteni and Colagrossi [1] and Antuono et al. [2] is here introduced. The transition between the two models is driven by a variable parameter introduced in the diffusive term. The dynamic pressures acting on the body profile of the breakwaters are evaluated through a Moving Least Squares interpolator of neighbors fluid particles.

The proposed hybrid approach is firstly applied to simulate the interaction between regular waves and a vertical breakwater and, successively, for two types of perforated breakwaters. SPH results of dynamic pressures are compared with experimental data and the diffusive models by Molteni and Colagrossi [1] and Antuono et al. [2].

## II. PRELIMINARIES

The adopted governing equations of the flow evolution for the SPH model read as:

$$\left\{ \begin{array}{l} \rho_i \frac{D\mathbf{u}_i}{Dt} = - \sum_j (p_i + p_j) \nabla_i W_j(\mathbf{r}_i) V_j + \rho_i \mathbf{g}_i + \\ \quad + \alpha h c_0 \rho_0 \sum_j \frac{(\mathbf{u}_j - \mathbf{u}_i) \cdot \mathbf{r}_{ji}}{|\mathbf{r}_{ij}|^2} \nabla_i W_j(\mathbf{r}_i) V_j \\ \frac{D\rho_i}{Dt} = -\rho_i \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W_j(\mathbf{r}_i) V_j + D_i \\ p_i = c_0^2(\rho_i - \rho_0) \\ \frac{D\mathbf{r}_i}{Dt} = \mathbf{u}_i + \epsilon_X \sum_j (\mathbf{u}_j - \mathbf{u}_i) W_j(\mathbf{r}_i) V_j \end{array} \right. \quad (1)$$

where  $\mathbf{r}_{ji} = -\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ ,  $\mathbf{g}_i$  represents the mass force acting on the fluid, the symbols  $\rho_i$ ,  $p_i$ ,  $\mathbf{u}_i$  and  $V_i$  denote the  $i$ -th particle density, pressure, velocity and volume, and  $\rho_0$  and  $c_0$  are the initial density and sound speed, respectively. As regards

# Evaluation of SPH in capturing flow separation points on hydrophobic and hydrophilic bodies during bluff water entry

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**Abstract**— Water entry, where flow is generated from the impact of a body with the free-surface of a fluid, encompasses a broad range of problems, such as ship slamming and mine deployment. For such problems, the cavity formation behind the impacting body depends primarily on the Froude number, body geometry, and location of the flow separation from the body. For prescribed separation points, potential flow models can capture accurately the cavity kinematics until pinch-off [1]. For water entry of bodies with corners, where the separation points are fixed, SPH simulations [2] are also shown to capture the cavity kinematics. However, in contrast to bodies with corners, the location of the flow separation on bluff bodies is a priori unknown and depends, among other things, on the body surface [3]. For example, hydrophilic spheres below a threshold velocity produce no cavity while hydrophobic spheres always entrain air [3-5]. In [5,6] it is argued that the latter threshold velocity for a given body depends on fluid properties, such as viscosity and surface tension. This paper accesses the ability of weakly compressible SPH to capture the flow separation points on bluff bodies with hydrophilic and hydrophobic surfaces while investigating numerically the effect of the fluid properties. For the simulations we utilize a rationally modified weakly compressible SPH scheme (mSPH) [7], which regularizes instabilities due to the weak compressibility assumption and numerically dissipates spurious high frequency oscillations via spatial filtering, to obtain highly accurate and robust dynamics as well as kinematics for incompressible free-surface flows. The validity of the weak compressibility assumption is verified via a global error metric that quantifies the amplitude and temporal growth of the high frequency oscillations in the dynamics [8]. The effects of the hydrophobic and hydrophilic surface is modelled via imposing no-slip and free-slip kinematic boundary conditions on the body surface, following [3]. The body boundary conditions are enforced with the fixed ghost particle technique proposed in [9] where however, the density of the ghost particles is computed directly and independently of the pressure to ensure consistency with the governing equations and reduce the generation of high frequency oscillations. Viscosity and surface tension are modeled respectively following [9] and [10]. Validations with 2D experimental data are provided. Separation angles for hydrophobic cases are slightly under predicted with comparison to experiments. The challenges in capturing the separation points on hydrophilic points at lower Froude numbers are discussed.

## I. INTRODUCTION

Water entry characterizes a broad range of flows generated in various scientific and engineering applications: from Basilisk lizard water-walking to projectile deployment and ship slamming. For such problems both the kinematics of the air cavity formed behind the impacting body as well as the corresponding dynamics are still not well understood. The cavity formation is known to depend primarily on the Froude number, body geometry, and location of the flow separation from the body. For given Froude number, body geometry, and flow separation points potential flow models have been shown to capture the cavity kinematics with high accuracy [1]. Smoothed Particle Hydrodynamics (SPH) simulations have also been successful in simulating wedge water entry [2] where the separation points are fixed. However, for bluff bodies, in contrast to wedges, the location of the flow separation is a priori unknown. The latter is believed to be determined by complex smaller-scale physics influenced by viscosity, surface tension, and the body surface. For example, hydrophilic spheres below a threshold velocity produce no cavity while hydrophobic spheres always entrain air [3-5]. Moreover, in [5,6] it is argued that the latter threshold velocity for a given body depends on viscosity, surface tension, and surface smoothness. Therefore, it is unclear whether meso-scale, low-order numerical methods, such as SPH, can capture the kinematics of bluff water entry without user-prescribed location of the flow separation points. However, recent CFD results [3] have shown that modelling of hydrophobic and hydrophilic body surfaces with respectively simplified no-slip and free-slip body boundary conditions can capture the cavity kinematics of bluff water entry, even in the absence of surface tension. The scope of this paper is to assess the capability of SPH to capture the separation points of bluff water entry, similarly to (more complex and expensive) CFD methods.

SPH for incompressible, free-surface hydrodynamic flows [12] is a simple and efficient numerical technique often used for the simulation of violent flows, such as water entry and slamming, where there are few other alternatives. SPH is a Lagrangian method that owes its simplicity and efficiency to a

# Investigation of ship flooding situations by MPS and SPH methods compared to dedicated experiments

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**Abstract**—For realizing quantitative safety assessment of damaged ships, numerical simulation methods for predicted the dynamic behaviors of damaged ships are desired. In order to predict fast and largely-deformed free surface flows related to flooding, particle methods would be promising. In this study, systematic comparisons between the MPS and SPH methods, and a set of dedicated model experiments are performed on forced roll tests of two-dimensional and three-dimensional damaged car decks. Through the comparisons, capability of the particle methods for flooding problems are demonstrated and differences in prediction accuracy between the MPS and SPH methods are investigated. In addition, the three-dimensional effects of the flow evolution are then investigated.

## I. INTRODUCTION

Collision and grounding accidents of ships are frequently reported even nowadays when security issues are carefully looked by societies. Securing the survivability under flooding condition is one of the most important subjects in ship design. For quantitative safety assessment of the damaged ships, numerical simulation methods to predict the dynamic behaviors of damaged ships are desired, which enable simulating the ship motion from the beginning of water flooding to final equilibrium state. In order to predict fast and largely-deformed free surface flows related to flooding, e.g. progressive flooding, down flooding, and sloshing, particle methods would be promising. The authors applied the MPS (Moving Particle Semi-implicit) method [1], which can easily handle fragmentations and reconnections of free surface and can accurately follow interface deformations, to ship dynamic stability problems. Violent water flows coupled with nonlinear ship motions are well reproduced by system-based mathematical models coupled with the MPS [2][3].

In this study, systematic comparisons between the MPS and SPH (Smoothed Particle Hydrodynamics) [4][5] methods, and a set of dedicated model experiments are performed on forced roll tests of two-dimensional and three-dimensional damaged car decks. Through the comparisons, capability of the particle methods for flooding problems are demonstrated and differences in prediction accuracy between the MPS and SPH methods are investigated. In a first stage both methods are compared on 2-D situations without taking into account the air phase, showing discrepancies with the experiments. In a second stage, it is shown how modeling the trapped air in damaged compartments permits to recover closely the experimental results. This is done in two different ways: either by numerically modelling the local equations in both phases or by using a simple Boyle's law model. The three-dimensional effects of the flow evolution are then investigated using the MPS method.

## II. MPS AND SPH SOLVERS

### A. COMPS

The moving particle semi-implicit method was developed by Koshizuka and Oka [1] for solving incompressible fluids. The governing equations of the MPS method, dealing with incompressible fluid, are expressed as Eq.1-2. The first and second order differential operators in Eq.2 are calculated with discrete models called particle interaction models [1]. In the MPS method, the gravity and the viscous terms are solved explicitly and the Poisson equation for the pressure is solved implicitly.

In this study, COMPS (Computational code for Moving Particle Simulation) is used as the MPS solver. (See the

# Energy decomposition analysis in free-surface flows: road-map for the direct computation of wave breaking dissipation

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**Abstract**—A viscous free-surface flow energy decomposition analysis is conducted in the present paper. In the presence of a free surface, the viscous dissipation for a Newtonian liquid can be decomposed into two terms: an enstrophy component and a free-surface deformation component. Equations for such terms in the weakly compressible SPH (WCSPH) formalism are devised. They require the discretization of a volume and a surface integral, respectively. Applying energy conservation, a double-checking of the free surface term is developed and applied, confirming the quality of the surface integral SPH evaluation, even in the presence of moderately fragmented free surface. Application to a large amplitude standing wave with breaking is presented.

## I. INTRODUCTION

Breaking waves induced mechanical energy dissipation is important for the design of earthquake sloshing dampers for buildings and bridges. Its modelling is an extremely challenging problem with mesh based VOF techniques due to the diffusion at the fragmented interface. Sun & Fujino [1] looked at the topic by semi-empirical methods and Iafratti [2] analyzed the vorticity generation during dam-breaks. Bouscasse et al. [3], [4] demonstrated the importance of wave breaking dissipation in damping angular motions, by performing an analogy with a hydraulic jump. However, insight on the dissipation mechanisms due to breaking is yet an open problem.

Colagrossi et al. [5] conducted a decomposition analysis of mechanical energy dissipation contributors in small amplitude gravity waves. That analysis is pursued here by extending it to large amplitude waves with wave breaking and by directly evaluating the free surface terms through SPH summations.

The paper is organized as follows: physical problem, governing equations and boundary conditions are first presented; the dissipation sources are then individualized through volume and surface integrals; the implementation of these integrals in SPH is presented and applied to a standing wave, discussing the influence of its amplitude, the fluid viscosity and the onset of breaking influence. Finally some conclusions are drawn.

## II. PHYSICAL PROBLEM AND GOVERNING EQUATIONS

### A. Governing equations

A fluid domain  $\Omega$  is considered whose boundary,  $\partial\Omega$ , consists of a free surface,  $\partial\Omega_F$ , and of a solid boundary  $\partial\Omega_B$  (Fig. 1); in practical applications periodic boundaries may be also considered. Since WCSPH will be employed at the discrete level, compressible Navier-Stokes conservation equations are of application:

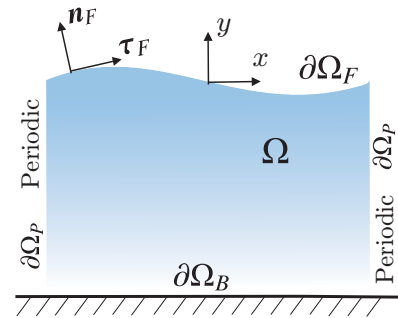


Fig. 1. Layout of the physical domain

$$\begin{cases} \frac{D\rho}{Dt} = -\rho \operatorname{div}(\mathbf{u}), \\ \frac{D\mathbf{u}}{Dt} = \mathbf{f} + \frac{\operatorname{div}(\mathbf{T})}{\rho}, \end{cases} \quad (\text{II.1})$$

where  $D/Dt$  represents the Lagrangian derivative,  $\mathbf{u}$  the flow velocity,  $\rho$  the fluid density,  $\mathbf{T}$  the stress tensor,  $\mathbf{D}$  the rate of strain tensor and  $\mathbf{f}$  is a generic specific body force. Thermal conductivity effects are here neglected. The pressure  $p$  is linked to density and internal energy through a state equation which changes depending on the nature of the fluid (gas or liquid). For example in the weakly-compressible regime for a liquid a simple adiabatic linear state equation can be used to link the pressure and density fields:

$$p = c_0^2 (\rho - \rho_0) \quad (\text{II.2})$$

# Smoothed Particle Hydrodynamics (SPH) simulation of a high-pressure homogenizer

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**Abstract**—A fully three-dimensional Smoothed Particle Hydrodynamics (SPH) code has been developed and validated with the objective to simulate primary atomization [1]. It is capable of simulating shear-driven and multi-phase incompressible flows, using the weakly compressible SPH approach. With this prerequisites the simulation of a generic high pressure homogenization orifice was conducted to show the ability of the code to simulate technical relevant interfacial problems. The results are compared to Micro Particle Image Velocimetry measurements, focusing on the velocity distribution of the continuous phase and the droplet deformation and disintegration. The findings demonstrate that the code is promising regarding the simulation of the prevailing high velocities and shear driven break-up.

## I. INTRODUCTION

Emulsification in high pressure homogenization (HPH) units is widely used, but still it is not possible to predict the droplet sizes and their distribution from system parameters, such as geometry, materials and process data. Therefore, the development and optimization of products is based on trial and error. Models to describe droplet disintegration and to estimate the resulting size distribution only exist for well defined boundary conditions, e.g. laminar shear and elongational flow [2]. But in the HPH the flow conditions mostly are superpositions of different flow types, which makes a prediction rather complex. In addition, cavitation could occur. A general mechanism was not found up to now [3], therefore models, which are based on averaged values [4], are developed. For the development of more sophisticated models it is necessary to characterize the flow conditions and the droplet break-up mechanisms in the HPH. This can be done using visual experiments [4], [5] or numerical predictions [6]–[8]. However the experimental analysis of the system by classical methods, e.g. measuring probes, as well as modern laser based diagnostics, like Micro Particle Image Velocimetry ( $\mu$ -PIV), is limited. This is due to the high flow velocity through very small geometries on one hand and the small droplet sizes on the other hand [9]. A detailed numerical investigation is time consuming due to the flow conditions, ranging from laminar to turbulent, and multi-phase phenomena.

In literature mostly grid-based numerical simulations with the  $k - \epsilon$  turbulence model are conducted. On one hand they are used to investigate the prevailing flow conditions for fast ge-

ometry optimization and as indicators for phenomena to look out for in experiments [8], [10]. On the other hand the most important parameters for theoretical models, the pressure loss  $\Delta p$  [11] and the dissipation rate of the turbulent kinetic energy  $\epsilon$  [7], can be determined. A different approach, which focuses on the investigation of the relevant flow conditions leading to droplet disintegration, as function of the pressure loss  $\Delta p$  can be found in [6]. There, a two-dimensional, multi-phase Direct Numerical Simulation (DNS) is conducted, whereas the multi-phase interaction is described by the Volume of Fluid (VoF) method using the Continuum Surface Force (CSF) model [12] with Piecewise Linear Interface Construction (PLIC). Such a reconstruction of the interface requires an enormous amount of computational effort. Furthermore, any inaccuracies of the interface reconstruction, causes an erroneous estimation of the interface curvature and, thus a wrong estimation of the surface tension force. As consequence, the whole disintegration process cannot be predicted accurately. Other existing methods have their drawbacks too, like the Level Set approach, which does not conserve mass strictly, or VoF methods with adaptive mesh refinement, which leads to high computational costs.

At this point the Smoothed Particle Hydrodynamics (SPH) method seems to be a promising alternative. Due to the Lagrangian frame of reference, the interface is advected inherently and complex geometries are handled naturally, because no mesh generation is required.

In this paper the ability of our SPH-code to simulate technical relevant interfacial problems, in this case a generic HPH process, is addressed. Therefore, generic two-dimensional simulations of an homogenization unit were conducted and compared to  $\mu$ -PIV experiments.

## II. SPH FORMULATIONS

Mathematical description of macroscopic flows is based on the continuum hypotheses for three dimensions. The Navier-Stokes equations as well as the conservation equation for mass and temperature have to be solved. To close the system of equations a suitable equation of state, which serves to couple the pressure  $p$  and the density  $\rho$ , has to be utilized.

# A semi-implicit SPH scheme for the shallow water equations

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**Abstract**—This work focuses on the development of a new semi-implicit SPH scheme for the shallow water equations, following the semi-implicit finite volume and finite difference approach of Casulli [1]. In standard explicit numerical methods, there is often a severe limitation on the time step due to the stability restriction imposed by the CFL condition. This paper proposes, a new semi-implicit SPH scheme, which leads to an unconditionally stable method. To this end, the discrete momentum equation is substituted into the discrete continuity equation to obtain a symmetric positive definite linear system for the free surface elevation. The resulting system can easily be solved by a matrix-free conjugate gradient method. Once the new free surface location is known, the velocity at the new time level can directly be computed and the particle positions can subsequently be updated. A simple and yet non-trivial 1D test problem for the 1D shallow water equation is presented.

## I. INTRODUCTION

This paper proposes a novel semi-implicit SPH scheme applied to the shallow water equations. We consider one-dimensional inviscid hydrostatic free surface flows. These flows are governed by the *shallow water equations* which we can derive from the three dimensional Navier-Stokes equations with the assumption of a hydrostatic pressure distribution (see [3], [11]).

A considerable amount of work has been done for both structured and unstructured meshes using finite difference, finite volume and finite element schemes ([3], [11], [17], [18], [19]). A major problem of explicit schemes in numerical methods is their severe time step restriction, where the Courant-Friedrichs-Lewy (CFL) condition imposes the time step size in terms of the wave propagation speed and the mesh size. Hence, the major advantage of a semi-implicit approach is that stable schemes are obtained which allow large time step sizes at a reasonable computational cost. In a staggered mesh approach for finite differences and volumes, discrete variables are often defined at different (staggered) locations. The pressure term, which is the free surface elevation is defined in the cell center while the velocity components are defined at the cell interfaces. In the momentum equation, pressure terms are due to the gradients in the free surface elevations and the velocity in the mass equation (i.e., free surface equation) are both

discretized implicitly whereas the nonlinear convective terms are discretized explicitly. The semi-Lagrangian method is one of the techniques to discretize these terms explicitly (see [12], [13], [14]).

In this paper a new semi-implicit *Smoothed Particle Hydrodynamics* (SPH) scheme for the numerical solution of the shallow water equations is proposed and derived. The flow variables in this present study are the particle free surface elevation, particle total water depth and the particle velocity. The discrete momentum equations are substituted into the discretized mass conservation equation to give a discrete equation for the free surface leading to a system in only one single scalar quantity, the free surface elevation location. The system is solved for each time step as a linear algebraic system. The components of the momentum equation at the new time level can be directly computed from the new free surface. This can be conveniently solved by a matrix-free version of the conjugate gradient (CG) algorithm [4]. Consequently, the particle velocities at the new time level are computed and the particle positions are updated. In this semi-implicit SPH method, the stability is independent of the wave celerity. Hence, a relatively large time steps can be permitted to enhance the numerical efficiency [3].

The remainder of this paper is structured as follows: In section II, the numerical models for the one-dimensional shallow water equations and models used for the particle approximations are presented. In section III, the key ideas of the proposed semi-implicit SPH scheme are presented and derived. One dimensional numerical results to validate the scheme are presented in section IV. Section V presents the concluding remarks and an outlook to future research.

## II. NUMERICAL MODEL

This section details the computational models and their accompanying particle approximations. Vectors are defined by reference to Cartesian coordinates. The latin subscript is used to identify particle locations, where subscripts  $i$  denotes the focal particle whereas the subscript  $j$  denotes the neighbor of particle  $i$ . Einstein's summation will be employed for repeated superscripts.



# Multiphase SPH for liquid-dust flow and its application to sedimentation in a turbulently convecting flow

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**Abstract**— This paper is concerned with the simulation of multiphase fluids where the phases are liquids and solid particles (we refer to them as dust hereafter) using the multiphase SPH model. First, by simulating the sedimentation of the dust in a static liquid, we show that SPH can be successfully applied to such problems. Second, we simulated the settling of particles in the presence of turbulence. Given that the sedimentation occurs within a very thin boundary layer which can hardly be resolved, we introduce a new sink model for sedimentation. From the result of turbulent settling simulation, we verified that our multiphase SPH model simulates turbulent settling very well.

## I. INTRODUCTION

This paper is concerned with the simulation of dusty liquid fluids using SPH. The SPH equations of motion of a dust-fluid system were first given by Monaghan and Kocharyan [1]. The algorithm was applied successfully to dusty disks of gas around stars [2] [3]. Laibe and Price [4], [5] improved the original formulation and applied the resulting algorithm to dust and gas in an astrophysical context. The results were in good agreement with theory.

In this paper we apply the algorithm to the case of dust in a liquid. The equations of motion are then those given by Harlow and Amsden [6], [7] and used by Valentine and Wohletz [8] for the simulation of volcanic dusty-gas eruptions. Closely related equations are those discussed by Gidaspow [9] and Kuipers et al. [10]. The sedimentation model is closely related to the analytic model by Martin and Nokes [11], [12].

We shall show that our SPH model can be successfully applied to the multi-phase problems where the phases are liquid and dust by simulating the motion of dust in a static liquid. Then, we show the simulation result of the sedimentation in the presence of turbulence using our multiphase SPH model. In a turbulently convecting flow, particles are stirred by the turbulence but they can sediment close to the bottom boundary where the no-slip boundary condition drives the particle velocity to zero. The layer of sediment is normally very thin, and to simulate it correctly requires a very large number of particles. To escape this problem we introduce a new SPH algorithm based on the idea that the boundary forms a sink. The continuum version of the

continuity equation therefore has an extra sink term that can be interpreted in an SPH formulation by allowing the SPH dust particles to lose mass in the neighbourhood of the sedimenting boundary. This algorithm enables us to simulate the sedimentation in the presence of turbulence without resolving the thin boundary layer.

## II. MODEL DESCRIPTION

### A. Equations of Motion

The equations for continuum analysis we used are those given by Harlow and Amsden [6], [7] and

$$\frac{d\hat{\rho}_l}{dt} = -\hat{\rho}_l \nabla \cdot \mathbf{v}_l \quad (1)$$

$$\frac{d\hat{\rho}_d}{dt} = -\hat{\rho}_d \nabla \cdot \mathbf{v}_d \quad (2)$$

$$\frac{d\mathbf{v}_l}{dt} = -\frac{\nabla P}{\rho_l} - \frac{K}{\hat{\rho}_l} (\mathbf{v}_l - \mathbf{v}_d) + \mathbf{g} \quad (3)$$

$$\frac{d\mathbf{v}_d}{dt} = -\frac{\nabla P}{\rho_d} - \frac{K}{\hat{\rho}_d} (\mathbf{v}_d - \mathbf{v}_l) + \mathbf{g} \quad (4)$$

where subscript  $l$  and  $d$  refer to the liquid and dust, respectively,  $P$  is the pressure,  $K$  is a drag factor,  $\mathbf{v}_l$  and  $\mathbf{v}_d$  are the liquid and dust velocities, respectively, and  $\mathbf{g}$  is the external self-gravity.  $\hat{\rho}_l$  and  $\hat{\rho}_d$  are the effective densities of each phase per unit volume of the mixture, and are related to  $\rho_l$  and  $\rho_d$ , the material densities of each phase by

$$\hat{\rho}_l = \theta_l \rho_l \quad (5)$$

$$\hat{\rho}_d = \theta_d \rho_d \quad (6)$$

# A Parallel SPH Implementation on Shared Memory Systems

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**Abstract**—We present a parallel implementation of SPH for shared memory computers. Our approach is based on domain decomposition and space filling curves (SFC). The particles are sorted and assigned to threads according to the Z-curve. This ensures per thread local storage of most frequently accessed data, avoids NUMA-unfriendly memory allocations, reduces data races and allows efficient calculation of symmetric inter-particle forces. We describe a simple and inexpensive dynamic load balancing algorithm. Finally, we present strong and weak scalability results of the implementation, and we identify sources of overhead.

## I. INTRODUCTION

The Smoothed Particle Hydrodynamics (SPH) method is currently used in many application areas including fluid dynamics, solid mechanics, astrophysics, coastal and marine engineering, and others. Compared to other simulation techniques, SPH simulations are computationally expensive: a large number of particles is required to achieve good accuracy; small time steps are needed, a limitation that results from utilizing explicit time integrators; interacting particles must be identified in every time step due to the particle movement. For that reason much attention has been paid to the parallelization of the method, mainly considering highly parallel systems, i.e. computer clusters and Graphic Processing Units (GPU). Examples are the open-source code DualSPHysics [1] (<http://www.dual.sphysics.org>) and the code SPH-flow [2] (<http://www.sph-flow.com>).

Although some work has been done on the parallelization of SPH on shared memory systems [3], [4], the attention to this type of architecture has been limited. However the number of cores per processors quickly increases, and will continue to increase. This, together with multi-socket boards provided with fast interconnects featuring cache-coherent non-uniform memory access (ccNUMA), provides shared memory system with large calculation power.

Despite the fact that a shared memory space suggests easier parallelization, there are several factors that are a detriment to efficiency. In particular, sharing of cache memory may lead to extra cache misses, and on systems with NUMA, improper data placement in memory can lead to significant latencies if threads often access data that reside far from them, possibly also causing bandwidth bottlenecks. Also, different

synchronization mechanisms may be required in order to avoid data races, which in turn introduces parallel overhead.

In the next section we briefly discuss modern shared memory architectures and describe a strategy to efficiently use caches and avoid NUMA-unfriendly memory allocations. Then we elaborate on the domain decomposition technique and the approach to handle data accesses at the boundary of the subdomains. Finally, we present and discuss the parallel algorithm. Section III presents a scalability study for a breaking dam problem, and we analyze the load balance during the different phases of the simulation loop.

## II. PARALLELIZATION ON SHARED MEMORY

In order to reduce the computational cost, SPH implementations exploit the compact condition that must be satisfied by the kernel, i.e. every particle interacts only with particles inside a local neighborhood with radius  $\kappa h$ , where  $\kappa$  is a constant that depends on the kernel function, and  $h$  is the smoothing distance. Different data structures can be used to efficiently identify interacting particles.

For simulations that discretize the physical domain using particles with (approximately) the same smoothing distance, the most efficient data structure is an underlying regular grid. Every cell in the grid has information regarding the particles that lay in it. The cell size is chosen so that interacting particles are only in direct neighboring cells. Then, the SPH simulation loop generally consist of the following steps:

- 1) assign particles to grid cells depending on their current position,
- 2) determine interacting particles using the information on the grid,
- 3) compute flux terms, i.e. process the interactions,
- 4) perform time integration.

Flux terms can be computed in two ways: (a) for every particle  $i$  find the list of neighbors and compute the contribution of  $i$ 's neighbors to  $i$ ; (b) find all interacting pairs of particles, then for every pair  $(i, j)$  account for the reciprocal contributions of particles  $i$  and  $j$ , exploiting the symmetry of the interactions.

The parallelization of the first approach is simple. It is an embarrassingly parallel algorithm given that every particle can

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