8th INTERNATIONAL SPHERIC WORKSHOP

Trondheim, June 4-6, 2013

EXCERPTS FROM PROCEEDINGS

This document contains the first page of all papers presented at the 8th SPHERIC workshop. For full papers, please contact corresponding authors.

8th International Smoothed Particle Hydrodynamics European Research Interest Community (SPHERIC) Workshop

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Program, Tuesday June 4

0800	**Registration**		
0830	**Opening of the 8th SPHERIC Workshop**		
0845	**Keynote**	**SPH - How I learnt to stop worrying and love Lagrangians**	**Daniel Price**
0935	**Session 1**	**Boundary treatment**	**Chair: David le Touzé**
	Paper 1-1	Application of the unified semi-analytical wall boundary conditions to incompressible SPH	A. Leroy, D. Violeau, M. Ferrand & C. Kassiotis
	Paper 1-2	SPH approximate Zeroth and First-order consistent boundary conditions for irregular boundaries	G. Fourtakas, R. Vacondio, & B. D. Rogers
	Paper 1-3	Consistency analysis of flow field extension models into ghost fluid regions for SPH solid body boundary condition implementations	P.E. Merino-Alonso, F. Macià, A. Souto-Iglesias & A. Colagrossi
	Paper 1-4	Semi-Analytical Conditions for Open Boundaries in Smoothed Particle Hydrodynamics	C. Kassiotis, M. Ferrand & D. Violeau
1040	**Coffee Break**		
1110	**Session 2**	**Theoretical & Numerical aspects of SPH**	**Chair: Damien Violeau**
	Paper 2-1	Waves and swimming bodies in a stratified fluid	J.J.Monaghan & J.B.Kajtar
	Paper 2-2	An improved corrective smoothed particle method approximation for second-order derivatives	S.P. Korzilius, W.H.A. Schilders & M.J.H. Anthonissen
	Paper 2-3	Pressure-corrected SPH with innovative particle regularization algorithms and non-uniform, initial particle distributions	P. H. L. Groenenboom & B. K. Cartwright
	Paper 2-4	A Simple and Effective Scheme for Dynamic Stabilization of Particle Methods	N. Tsuruta, A. Khayyer, H. Gotoh & H. Ikari
	Paper 2-5	An implicit SPH solution of the Burgers equation	L.M.González & J.L.Cercós
1230	**Lunch**		
1330	**Session 3**	**Multiphase**	**Chair: Joe Monaghan**
	Paper 3-1	A Novel Error-Minimizing Scheme to Enhance the Performance of Compressible-Incompressible Multiphase Projection-Based Particle Methods	A. Khayyer, H. Gotoh, H. Ikari & N. Tsuruta
	Paper 3-2	A generalized SPH-DEM discretization for the modelling of complex multiphasic free surface flows	R.Canelas, A. Crespo, J.Domínguez, & R.M.L.Ferreira
	Paper 3-3	Modelling of Phase Decomposition Using a Fourth-Order Derivation for SPH	M. Hirschler, M. Huber, W. Säckel & U. Nieken
	Paper 3-4	The SPH Modeling of the Deformation of a Droplet under the Effect of Constant External Electric Field	A. Rahmat, M.S Shadloo & M. Yildiz
1435	**Session 4**	**Coupled Methods**	**Chair: Paul Groenenboom**
	Paper 4-1	Multi-purpose interfaces for coupling SPH with other solvers	B. Bouscasse, S. Marrone, A. Colagrossi & A. Di Mascio
	Paper 4-2	Coupling of a SPH-ALE and a Finite Volume Method	M. Neuhauser, F. Leboeuf, J.-C. Marongiu, M. Rentschler, & E. Parkinson
	Paper 4-3	On the use of particle based methods for cosmological hydrodynamical simulations	M. Schaller, R. G. Bower & T. Theuns
1535	**Coffee Break**		
1600	**Session 5**	**Turbulence**	**Chair: Andrea Colagrossi**
	Paper 5-1	Density diffusion terms and solid wall models in weakly compressible SPH	A.Valizadeh & J.Monaghan
	Paper 5-2	SPH hyperviscosity model for incompressible turbulence	Y.L. Shi, M. Ellero and N.A. Adams
	Paper 5-3	Direct numerical simulation of 3-D turbulent wall bounded flows with SPH	A. Mayrhofer, D. Laurence, B. D. Rogers, D. Violeau & M. Ferrand
1700	**Discussion**	**Grand Challenges of SPH**	**Damien Violeau & Ben Rogers**
1800	**Reception**		

Program, Wednesday June 5

0830	**Keynote**	**Numerical Stability of SPH for Weakly Compressible Viscous Flows: Optimal Time-Stepping**	**Damien Violeau**
0920	**Session 6**	**Free surface & interface modelling**	**Chair: Antonio Souto-Iglesias**
	Paper 6-1	SPH modelling of 3D body transport in free surface flows	A. Amicarelli, R. Albano, D. Mirauda, G. Agate, A. Sole, & R. Guandalini
	Paper 6-2	Application of SPH on study of a deep water plunging wave	M. H. Dao & E. S. Chan
	Paper 6-3	SPH surface tension model without need for calibration or evaluation of curvature	A.C.H. Kruisbrink, F.R. Pearce, T. Yue, H.P. Morvan & K.A. Cliffe
	Paper 6-4	Volume reformulation of spatially varying interactions using the example of moving contact lines for a complete surface tension description	M. Huber, W. Säckel, M. Hirschler, U. Nieken & S. M. Hassanizadeh
1025	**Coffee Break**		
1055	**Session 7**	**Theoretical & Numerical aspects of SPH**	**Chair: Xiangyu Hu**
	Paper 7-1	Several approaches to achieve better accuracy of a single precision SPH code	V.Titarenko, B.D.Rogers & A.Revell
	Paper 7-2	Measures of Particle Disorder	M.Antuono, A.Colagrossi, S.Marrone &B.Bouscasse
	Paper 7-3	A Switch for Artificial Resistivity and Other Dissipation Terms	T.S.Tricco & D.J.Price
	Paper 7-4	Accuracy and performance of implicit projection methods for transient viscous flows using SPH	N.Trask & M.Maxey
	Paper 7-5	PySPH: A Python framework for SPH	K.Puri, P. Ramachandran, P.Pandey, C.Kaushik & P.Godbole
1215	**Lunch**		
1315	**Session 8**	**Multi-resolution techniques**	**Chair: Ben Rogers**
	Paper 8-1	Particle refinement and derefinement procedure applied to Smoothed Particle Hydrodynamics method	D. A. Barcarolo, D. le Touzé, G. Oger & F. de Vuyst
	Paper 8-2	A multiscale SPH modeling of near-wall dynamics of leukocytes in flow	B.Gholami, A.Comerford & M.Ellero
	Paper 8-3	Shock interactions with dusty gases using multi-phase RSPH	M. G. Omang & J. K. Trulsen
	Paper 8-4	SWIFT: Fast algorithms for multi-resolution SPH on multi-core architectures	P.Gonnet, M.Schallery, T.Theunsyz & A.B. G. Chalk
1420	**Session 9**	**High Performance Computing**	**Chair: Daniel Price**
	Paper 9-1	FPM Flow Simulations Using an Adaptive Domain Decomposition Strategy	C. Vessaz, E. Jahanbakhsh, M. Reclari and F. Avellan
	Paper 9-2	Integration Of Spring Physics With The SPH Method For Quasi-Solid To Fluid Interaction Using GPGPU Programming	S.M.Longshaw, B.D.Rogers & P.K.Stansby
	Paper 9-3	AQUAgpusph, a free 3D SPH solver accelerated with OpenCL	J.L. Cercos-Pita, A. Souto-Iglesias, L.M. Gonzalez, F. Macià
	Paper 9-4	Simulating more than 1 billion SPH particles using GPU hardware acceleration	J.M. Domínguez, A.J.C. Crespo, B.D. Rogers & M. Gomez-Gesteira
1525	**Coffee Break**		
1550	**Session 10**	**Solids & Structural Mechanics**	**Chair: Paal Skjetne**
	Paper 10-1	The Way to an Enhanced Smoothed Particle Hydrodynamics Formulation Suitable for Machining Process Simulations	F.Spreng & P.Eberhard
	Paper 10-2	Shock loading of layered materials with SPH	I.Zisis & B.van der Linden
	Paper 10-3	SPH Simulations of Abrasive Processes at a Microscopic Scale	C. Nutto, C. Bierwisch, H. Lagger & M. Moseler
1630	**Steering Committee Meeting**		
1800	**Workshop Banquet**		

Program, Thursday June 6

0900	**Session 11**	**Maritime applications**	**Chair: Peter Stansby**
	Paper 11-1	SPH modelling of the flow field with spilling generated by a hydrofoil	S.Sibilla, D. D.Padova & M.Mossa
	Paper 11-2	Slam Modelling with SPH: The Importance of Air	S. J. Lind, P. K. Stansby, B. D. Rogers
	Paper 11-3	Comparison of SPH and VOF simulations with experimental measured wave-induced impact loads due to Green Water Events	C.Pakozdi & SINTEF SPH Team
	Paper 11-4	Simulation of extreme waves impacts on a FLNG	P.-M. Guilcher,J. Candelier,L. Béguin, G. Ducrozet & D. Le Touzé
1005	**Coffee Break**		
1020	**Session 12**	**Multiphase**	**Chair: Stefano Sibilla**
	Paper 12-1	Modelling Sediment Resuspension in Industrial Tanks using SPH on GPUs	G. Fourtakas, B. D. Rogers, D. Laurence
	Paper 12-2	GPU Acceleration of 3-D Multi-phase SPH Simulations for Violent Hydrodynamics	A.Mokos, B.D.Rogers,P.K.Stansby,J.M.Dominguez
	Paper 12-3	SPH Modelling of Bed Erosion for Water/Soil-Interaction	M.Leonardi & T.Rung
	Paper 12-4	A pool boiling model with SPH	S.Litvinov, D.Gaudlitz &X.Hu, N. Adams
1125	**Session 13**	**Exotic applications and methods**	**Chair: Thomas Rung**
	Paper 13-1	Application of Modified SPH to Quantum Mechanical Problems	S.Sugimoto, Y.Zempo
	Paper 13-2	Simulation of particulate suspensions with SPH and application to tape casting processes	P. Polfer, T. Kraft
	Paper 13-3	SmoothViz: An Interactive Visual Analysis System for SPH Data	V. Molchanov, A.Fofonov, S.Rosswog, P.Rosenthal & L.Linsen
	Paper 13-4	<MPS> ≡ <SPH>	F. Macià, A. Souto-Iglesias, L. M. González & J.L. Cercos-Pita
1230	**Lunch**		
1330	**Session 14**	**Turbulence**	**Chair: Jean-Christophe Marongiu**
	Paper 14-1	A transport-velocity formulation for Smoothed Particle Hydrodynamics	S. Adami, X.Y. Hu & N.A. Adams
	Paper 14-2	SPH simulations of elastic turbulence and mixing in a periodic channel flow	M.Grilli, A.Vazquez-Quesada & M.Ellero
	Paper 14-3	Simulating 3D turbulence with SPH	S. Adami, X. Y. Hu and N. A. Adams
1430	**Session 15**	**High Performance Computing**	**Chair: Abbas Khayyer**
	Paper 15-1	Dynamic Load-Balancing for Parallel Smooth Particle Hydrodynamics	P.Godbole, K.Puri & P.Ramachandran
	Paper 15-2	Effective memory layout and accesses for the SPH method on the GPU	K.O.Lye, C.Dyken, J.Seland & SINTEF SPH Team
	Paper 15-3	Efficient Massive Parallelisation for Incompressible Smoothed Particle Hydrodynamics with 10^8 Particles	X.Guo, S. Lind, B. D. Rogers, P. K. Stansby, M. Ashworth
1525	**Closing and Awards**		
1545	**Coffee and Goodbye**		

Application of the unified semi-analytical wall boundary conditions to 2-D incompressible SPH

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***Abstract*—This work aims at improving an incompressible SPH model (ISPH) by adapting to it the unified semi-analytical wall boundary conditions proposed by Ferrand *et al.* [1]. The ISPH algorithm considered is the one proposed by Lind *et al.* [2]. The new description of the wall boundaries allows to impose accurately a von Neumann boundary condition on the pressure that corresponds to the impermeability condition. The shifting and free-surface detection algorithms are adapted to the new boundary conditions. A new way to compute the wall renormalisation factor in the frame of the unified semi-analytical boundary conditions is proposed in order to decrease the computational time. We propose several 2-D verifications to the present approach. Our results were compared to analytical or other numerical results. We investigated the convergence of the method and proved its ability to model complex free-surface and turbulent flows. The results were generally improved compared to a weakly compressible SPH model with the same boundary conditions, especially in terms of pressure prediction, with a lower computational time.**

I. Introduction

Modelling incompressible flows with the SPH method has classically been done through weakly compressible SPH (WCSPH) models, as is thoroughly described in [3]. In this case, the pressure is calculated through an equation of state, which causes the pressure prediction to be noisy and, in many cases, inaccurate. To remedy this issue, truly incompressible approaches (ISPH) were developed [4]–[6]. Amongst the ISPH methods, the one consisting in imposing a divergence-free velocity field while stabilizing the simulation through a particle shift was shown to produce accurate results while reducing the computational time compared to a WCSPH model [7]. Thus, we chose this model as a starting point for a new ISPH model where boundary conditions would be imposed accurately. Most available ISPH models in the literature are based on ghost particles or mirror particles [2], [7], [8], which lead to approximate boundary conditions that can hardly be extended to complex geometries. This is a serious issue, since the proper imposition of pressure boundary conditions is crucial when solving the pressure Poisson equation. Recently, wall-boundary models were proposed that account for the kernel truncation close to the wall through the application of a renormalisation factor in the discrete interpolation formula. In particular, Ferrand *et al.* [1] proposed a way of computing the renormalisation factor semi-analytically together with a new formulation of the differential operators, which proved to be very accurate even close to the walls. The new formulation of the Laplacian operator allows the imposition of boundary conditions in a natural way. This was applied to the $k-\epsilon$ turbulence model where Neumann boundary conditions could be prescribed accurately on k and ϵ. Associating the wall boundary conditions proposed by Ferrand *et al.* [1] to an ISPH model will allow to impose accurately Neumann (or Dirichlet) boundary conditions on the pressure, being thus able to model properly flows presenting complex boundary geometries while taking advantage of the ISPH method. This is the aim of the present work. From now on these boundary conditions will be referred to as unified semi-analytical wall boundary conditions.

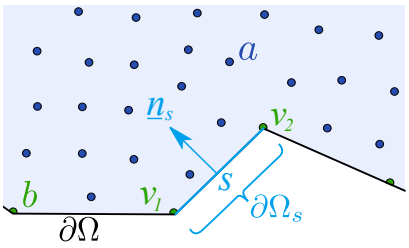

Fig. 1. Sketch of the different entities involved in the representation of the unified semi-analytical wall boundary conditions.

II. SPH interpolation in the frame of unified semi-analytical wall boundary conditions

Fluid particles which do not belong to a boundary are called here free particles. Solid boundaries in the method proposed by Ferrand *et al.* [1] are modelled by vertex particles $v \in V$ (see Fig. 1), which are fluid particles whose velocity is imposed to be equal to the one of the wall. They are linked together by segments $s \in S$, which compose a mesh of the boundary. The set of all fluid particles, including free and vertex particles, is noted P and particles belonging to $P = F \cup V$ will be noted a or b in what follows. The $5th$ order Wendland kernel [9] was used with $h = 2\delta r$ for all the simulations, where h is the smoothing length and δr is the initial interparticular space. With the boundary conditions used in this work, the discrete

SPH approximate Zeroth and First-order consistent boundary conditions for irregular boundaries

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***Abstract*— In this paper a method to impose wall boundary conditions is presented. The wall is discretized by means of a set of virtual particles and is simulated by a local point symmetry approach. The extension of MVBP method guarantees that arbitrarily complex domains can be readily discretized guaranteeing approximate zeroth and first order consistency. The extended MVBP model is demonstrated for cases including hydrostatic conditions for still water in a tank with a wedge and for curved boundaries, where significant improved behaviour is obtained in comparison with the conventional boundary techniques. Finally the capability of the numerical scheme to simulate a dam break simulation is also shown.**

I. INTRODUCTION

Due to the intrinsic nature of kernel based interpolation and to the Lagrangian approach, imposing boundary conditions in SPH is still an open problem. The approach proposed by Monaghan [11, 14] 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.

Mirror or ghost particles as introduced by Randles and Libersky [16] is another widely used way to describe boundaries in SPH [2, 9]. Kulasegaram et al. [7] 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 to approximate the force originating from variational principles. The idea was further developed in [1, 3-4]. These methods have the advantage of restoring zero-consistency in the SPH interpolation but the discretization of complex 3D geometries and/or multiphase flows is not straightforward. In general, the repulsive force method is more flexible because it can be used to describe complex moving boundaries, but it can introduce a non-physical pressure oscillation and it does not reduce the effect of kernel truncation near the wall.

Ferrari et al. [1] proposed a local point symmetry (as opposed to ghost particles) 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) [19]. In this work this method is further enhanced in order to assure approximate first order consistency in presence of arbitrarily complex boundaries.

The paper is organized as follows; in section II the governing equations are briefly recalled, in section III the novel extended Modified Virtual Boundary Particle method is presented and finally in Section IV the numerical scheme is tested against analytical and reference solutions.

II. GOVERNING EQUATIONS

This section presents the governing equation in SPH form. Throughout this paper, superscripts α and β denote the Cartesian coordinates using Einstein's summation and i and j the interpolated particle and its neighbours respectively. The density evolution and momentum of the particles follow the Navier-Stokes equations [12]

$$\begin{cases} \dfrac{d\rho_i}{dt} = \sum_j^N m_j u_{ij}^{\beta} \dfrac{\partial W_{ij}}{\partial x_i^{\beta}} \\ \dfrac{du_i^{\alpha}}{dt} = \sum_j^N m_j \left(\dfrac{P_j}{\rho_j^2} + \dfrac{P_i}{\rho_i^2} + \Pi_{ij} \right) \dfrac{\partial W_{ij}}{\partial x_i^{\alpha}} + g_i^{\alpha} \\ \dfrac{dx_i^{\alpha}}{dt} = u_i^{a} \end{cases}, \qquad (1)$$

where x_i^{α} is the position , u_i^{α} is the velocity , ρ is the density , P is the pressure, m is the mass and g_i^{α} is the gravity acceleration. In this paper, the Wendland kernel [20] has been used as a smoothing function but numerical test has shown similar results with other kernels such as the cubic spline. Also, artificial viscosity [12] has been used denoted as Π_{ij},

$$\Pi_{ij} = \begin{cases} \dfrac{-\alpha_{\pi} \overline{c_{ij}}}{\overline{\rho_{ij}}} \dfrac{h u_{ij}^{\beta} x_{ij}^{\beta}}{x_{ij}^{\beta 2}} & u_{ij}^{\beta} r_{ij}^{\beta} < 0 \\ 0 & u_{ij}^{\beta} r_{ij}^{\beta} \geq 0 \end{cases}, \qquad (2)$$

where α_{π} is the free parameter depending on each problem, the overbar denotes the average values of the i and j particles for the numerical speed of sound and density, $u_{ij} = u_i - u_j$ and $x_{ij} = x_i - x_j$. In the present study, weakly compressible SPH (WCSPH)

Consistency analysis of flow field extension models into ghost fluid regions for SPH solid body boundary condition implementations

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***Abstract*—In the present paper, the consistency of continuous SPH approximations to the differential operators appearing in the Navier-Stokes system is analyzed. In particular, emphasis is made on the consistency of such operators when evaluated close to the boundaries of the fluid domain and flow extension techniques are applied. The divergence of the velocity field, the pressure gradient and the velocity Laplacian, present in Navier-Stokes equations, are considered. The question of how the extension scheme used in each field, both velocity and pressure, may affect the accuracy of the SPH approximation of differential operators close to the boundaries is addressed. An answer to this question is given by means of consistency arguments based on analytical tools.**

I. Motivation

Flow extension models [1], [2], boundary-particle techniques [3], and boundary integral-based corrected formulations [4]–[6] are the most popular means to implement solid boundary conditions in SPH.

In [2] it was demonstrated that the integral SPH approximation, for unidirectional flows, to the Laplacian of the velocity field was only correct for a modified Takeda [7] extension of the flow fields into the ghost fluid region. However, no attention was paid to the divergence of the velocity, the pressure gradient or the case of flows with 2 velocity components. The analysis of [2] relies on a consistency analysis based on analytical tools.

In [8] it was shown that different mirroring schemes should be used when computing the divergence and the Laplacian of the velocity field. That analysis is based on energy conservation considerations.

The methodology of [2] will be herein extended to the divergence and gradient operators; it will be shown that the results of De Leffe et al. [8] for the divergence can be deduced from a consistency-based analysis. A similar methodology will be applied in this paper to pressure fields of any kind with emphasis on hydrostatic ones.

This paper is organized as follows: first, the governing equations of the physical problem are presented. Secondly, the flow fields are mathematically defined and an explanation of their form is given. Then, the notation for kernels and SPH methodology, including mirroring extensions, is presented. The SPH approximation of differential operators used in the present paper is also established. Next, cases in which SPH approximations do not give the correct value for the corresponding operators is given, and the consistency of general SPH approximations for the operators under consideration is studied. Finally, the results are discussed and lines for future work oriented in these directions are given.

II. Governing equations

The flow is modelled with the compressible Navier-Stokes equations (to be discretized using weakly compressible SPH) for a barotropic fluid in Lagrangian formalism:

$$\frac{D\rho}{Dt} = -\rho\,\nabla\cdot\mathbf{u}\,, \tag{1}$$

$$\frac{D\mathbf{u}}{Dt} = \boldsymbol{g} - \frac{\nabla P}{\rho} + 2\mu\nabla^2\mathbf{u}\,, \tag{2}$$

$$P := P(\rho,\rho_0,c_0)\,. \tag{3}$$

Here, ρ and μ are the fluid density and dynamic viscosity respectively, ρ_0 is the initial density, P is the pressure, c_0 is the sound velocity (assumed constant) and $\boldsymbol{g}$ is a generic external volumetric force field. The equation of state (3) can take different forms in the SPH context [9]. The flow velocity, $\mathbf{u}$, is defined as the material derivative of a fluid particle position $\mathbf{r}$:

$$\mathbf{u} := \frac{D\mathbf{r}}{Dt}. \tag{4}$$

III. Flow fields

A. Velocity field

We will consider a stream function of the form:

$$\psi(x_1,x_2) := G(x_1)H(x_2), \tag{5}$$

where both G and H are general C^∞ functions.

Semi-Analytical Conditions for Open Boundaries in Smoothed Particle Hydrodynamics

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***Abstract*—Due to the Lagrangian nature of SPH, treating inlet/outlet (that are intrinsically Eulerian) is a challenging issue. We investigate here an extension to open boundaries of the Unified Semi-Analytical conditions proposed in [1]. The main advantages of the present method are the quality of the fields obtained near the open boundary and the possibility to treat complex shapes. The method is implemented on a GPU fork of GPU-SPH [2]. We propose simple test cases to illustrate the performances of the proposed method and show some more complex problems like generation of waves without paddle and radiative outlet. The extension to 3-D is straightforward and an example is given as well.**

I. Introduction

The intrinsic computational cost of SPH makes natural the interest in simulations where only a part of a larger problem is treated. More generally, open boundaries are required in a lot of fluid mechanics problems. For this kind of simulation, inlet/outlet conditions need to be developed. Efficient inlet/outlet boundary treatment is also required when solving coupled problems, especially when strong coupling algorithms are used, since the fields near the open boundaries are exchanged between the coupled models, and perturbations can lead to instabilities [3]. The simplest way to treat inlet/outlet in SPH is to use a buffer layer, where the values of the fields at the boundary are imposed on several layers of particles that complete the kernel support of free particles close to the open boundary [4]. In the inlet case, when entering the fluid domain a buffer particle is marked as fluid particle and is then free to move. This sudden modification can generate spurious shocks. Using Riemann solvers can partially solve this issue [5], but treating complex inlet where the flow is non parallel to the normal of the boundary remains a difficult issue. Similarly, a fluid particle leaving the domain through an outlet is fisrt marked as a buffer particle, and some of its physical quantities are suddenly prescribed, generating shocks.

The Unified Semi-Analytical strategy proposed in [1] has shown promising results to treat both Dirichlet and Neumann conditions for wall boundary treatment in SPH. In this approach, the boundaries are discretized using boundary elements hereafter referred to as 'segments', as well as 'vertex' particles at their intersections. We propose here to extend this treatment to open boundaries. For this purpose, the main novelties are:

- two additional terms in the continuity equation, naturally derived the Unified Semi-Analytical approach;
- the masses of vertex particles evolve over time according to the desired mass flux at the connected segments;
- the vertex particles are used to create or delete fluid particles which are free to move.

All this changes make the formulation able to treat particles entering and leaving the domain without perturbations of the fields.

The outline of the paper is as follows: we first shortly describe in Section II the Unified Semi-Analytical boundary conditions for walls as proposed in [1], and extend it for inlet/outlet in Section III. In Section IV we explain how we handle a varying number of particles in our GPU implementation. In Section V we exhibit some numerical experiments to illustrate the ability of our method to treat wall-bounded and free-surface flows with complex inlet/outlet.

II. Semi-analytical *SPH* formulations for a weakly compressible Newtonian fluid

A. Space discretization

As illustrated in Figure 1, the weakly compressible Newtonian fluid domain Ω is discretised by a set of fluid particles $\mathcal{F}$ denoted by the subscripts $(.)_a$ and $(.)_b$, while the boundaries $\partial\Omega$ are discretized by a set of vertex particles $\mathcal{V}$ denoted by $(.)_v$ and connected to boundary segments $\mathcal{S}$ denoted by $(.)_s$. Each element stores information such as mass m_a, position center $\boldsymbol{r}_a$, Lagrangian velocity $\boldsymbol{v}_a$ (*i.e.* the Lagrangian derivative of the position), Eulerian fluid velocity $\boldsymbol{u}_a$ and density ρ_a and pressure p_a, as well as the volume $V_a = \frac{m_a}{\rho_a}$. It is important to underline that we need two discrete velocity fields, since the vertex particles and boundary segments are fixed in space but carry an

Waves and swimming bodies in a stratified fluid

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***Abstract*—There are fascinating possibilities for the application of SPH to zoological and biological problems where fluids, solids and elastic bodies move within irregular boundaries. One example is the application of SPH to the swimming of fish modelled by a system of linked-rigid bodies immersed in water (Kajtar and Monaghan 2008, 2010, 2012). Our studies of this system have involved a combination of rigid and elastic bodies moving in a domain with periodic, free and rigid boundaries. The ease of setting up a such a complex model, including motion near a free surface, is an advantage of SPH. In the present paper we consider the motion of the linked bodies in a stratified medium for which, as far as we are aware, no tests have been previously performed. In order to mimic the behaviour of fish the linked bodies oscillate at a frequency that is much higher than that of the normal modes of the interface. There is therefore little point in testing SPH by simulating the linearised modes of the interface. Instead, we estimate the accuracy of the SPH method by simulating the fluid motion when a suitable oscillating external force field is imposed on the fluid. Our results show that SPH gives good results for this class of problem. Combined with our previous results for the motion of linked bodies we can predict the effects of stratification on swimming and decide whether it is better to swim below or above the interface of a stratified fluid.**

I. Introduction

The present paper is primarily concerned with the accuracy of an SPH simulation of swimming bodies when the tank is stratified in two layers. Preliminary results were described at the Hamburg SPHERIC meeting, but they were not completed at that time because we did not have satisfactory tests of our simulations. In the present paper we consider the simulation of an analytical model supplemented by convergence calculations. The simplest analytical problem associated with a stratified tank, is the weakly perturbed motion generated by the disturbance of the interface for which the modal structure is well known (Lamb 1932). However, this classical problem is not relevant to the dynamics produced by the oscillating swimmer because the swimmer drives the motion, and does so at a frequency that is much greater than that of the normal modes for the typical density differences between the layers. To escape this difficulty we considered a novel test case where the stratified fluid is driven by an external force concentrated at the interface. An analytical solution can be found if the spatial structure of this force is based on the normal modes. The end result is that the motion is a combination of the normal modes plus the driven motion in much the same way as a driven simple harmonic oscillator. This makes the motion more realistic, but more complicated than a simple mode and provides a more demanding test. It is convenient to choose initial conditions where the perturbation and velocity of the interface are zero.

The unperturbed fluid consists of two horizontal layers, under gravity and a driving force. Each layer has thickness D. The velocity is assumed to be irrotational and the velocity $\mathbf{v}$ can therefore be written $-\nabla\Psi$. Because of the incompressibility condition $\nabla\cdot\mathbf{v}=0$ and $\nabla^2\Psi=0$. The force/mass is curl free and given by $-\nabla\Phi$. The variables in the upper layer, where the density is ρ', are denoted by Ψ' and Φ', and in the lower layer they are ρ, Ψ and Φ. We assume $\rho>\rho'$ so that the fluid is stable. We use a cartesian coordinate system with the x axis parallel to the unperturbed interface, and the origin of the coordinate system is at the interface. The upper and lower boundaries are rigid, and the viscous condition is free slip. The system is periodic in the x direction.

In the absence of external forces apart from gravity the velocity potentials have the form (Lamb 1932)

$$\Psi = K\sin(\bar\omega t+\beta)\sin(kx)\cosh k(y+D), \quad (1)$$

$$\Psi' = K'\sin(\bar\omega t+\beta)\sin(kx)\cosh k(y-D), \quad (2)$$

where K, K' and β are arbitrary constants and k is the wave number. The frequency $\bar\omega$ is given by the dispersion relation

$$\bar\omega^2 = gk\tanh(kD)\frac{(\rho-\rho')}{(\rho+\rho')}. \quad (3)$$

Guided by the form of the velocity potentials we consider the motion produced by the combination of gravity and the driving force potential

$$\Phi = \alpha\sin(\omega t)\sin(kx)\cosh k(y+D), \quad (4)$$

$$\Phi' = -\alpha\sin(\omega t)\sin(kx)\cosh k(y-D), \quad (5)$$

where α is a constant. The y component of the force is continuous at the interface (where $y=0$), and vanishes at the upper and lower boundaries. Note that the force is concentrated at the interface and falls off exponentially with the length scale $1/k$.

The fluid dynamical problem is then similar to that of a driven simple harmonic oscillator for which the solution consists of a general solution of the homogeneous equation (the solution in the absence of the driving force), together with a particular solution that satisfies the equation of motion with the driving force. With this in mind a suitable velocity potential satisfying $\nabla^2\Psi=0$ is given by

An improved corrective smoothed particle method approximation for second-order derivatives

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Abstract

To solve (partial) differential equations it is necessary to have good numerical approximations. In SPH, most approximations suffer from the presence of boundaries. In this work a new approximation for the second-order derivative is derived and numerically compared with two other approximation methods for a simple test case. The new method is slightly more expensive, but leads to a significantly improved accuracy.

I INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) is a numerical method for solving partial differential equations. It is a mesh-free, Lagrangian method in which the state of the system is represented by a finite set of particles. Although SPH was originally developed to solve astrophysical problems [5, 7] in which boundaries are not present, the method has attracted attention in other areas like fluid and solid mechanics. This has led to significant extensions and improvements to the original method [1].

However, in many areas the presence of boundaries is still leading to inaccurate approximations. This also holds for the second-order derivative. The original SPH approximation for the second-order derivative includes the second-order derivative of the kernel function, which is very sensitive to particle disorder [2, 10]. Therefore alternatives based on the first-order derivative [2] of the kernel function and the kernel function itself [4] have been proposed. Also it is suggested to include boundary terms in the approximation [8].

In this work we will consider the methods described in [4] and [8], as well as an improved version of the one in [4]. A one-dimensional setting will be assumed throughout this work. We will start by stating the kernel function we use, whereafter all three methods are briefly explained. The numerical comparison of the methods focuses on both uniformly and non-uniformly distributed particles.

II WENDLAND KERNEL

There are several options for the kernel function. Originally a Gaussian function was used [5]. A disadvantage of this function is that it does not have compact support, which is computationally more expensive. Other examples are a truncated Gaussian or B-spline functions. A short overview is given in [6]. Throughout this work we will use the Wendland kernel of fifth degree [9,13], given by:

$$W_h(x-y) = \alpha_{\mathrm{d}} \cdot \begin{cases} (2-|q|)^5 \left(2|q|^2 + \frac{5}{2}|q| + 1\right) & \text{for } |q| < 2, \\ 0 & \text{for } |q| \geq 2, \end{cases}$$

where h is the smoothing length, $\alpha_{\mathrm{d}} = 3/(128h)$ is a normalizing and spatial-dimension-dependent factor and $q = (x-y)/h$. The first-order derivative with respect to y of this function is given by:

$$W_h'(x-y) = \frac{7\alpha_{\mathrm{d}}}{h} \cdot \begin{cases} q(2-|q|)^4 (2|q|+1) & \text{for } |q| < 2, \\ 0 & \text{for } |q| \geq 2. \end{cases}$$

Since $\alpha_{\mathrm{d}} = \mathcal{O}(h^{-1})$ and $q = \mathcal{O}(h^0)$ as $h \to 0$, it follows that for this kernel we have:

$$W_h(x-y) = \mathcal{O}(h^{-1}) \quad \text{as} \quad h \to 0, \tag{1}$$
$$W_h'(x-y) = \mathcal{O}(h^{-2}) \quad \text{as} \quad h \to 0. \tag{2}$$

These orders play an important role in the accuracy of the kernel approximations. In the following sections we will consider several SPH approximations for the second-order derivative. In the accuracy analysis of these approximations we will implicitly use equations (1) and (2).

III APPROXIMATING A FIRST-ORDER DERIVATIVE

Before considering second-order derivatives, let us first have a look at the first-order derivative approximation. We will need this approximation later. In SPH, most approximations can be derived from the well-known Taylor series expansion of a function f around a point x:

$$f(y) = f(x) + (y-x)f'(x) + \frac{(y-x)^2}{2} f''(x) + \dots \tag{3}$$

To find the value of the derivative at x, we could start by subtracting $f(x)$ from both sides of the equation. Multiplying the entire equation with the odd function W_h' and integrating over the computational domain $\Omega := [x_\ell, x_{\mathrm{r}}]$ then gives:

$$\int_\Omega (f(y) - f(x))\, W_h'(x-y)\, \mathrm{d}y = f'(x) \int_\Omega (y-x) W_h'(x-y)\, \mathrm{d}y + \mathcal{O}(h).$$

For x satisfying $[x-2h, x+2h] \subset \Omega$ this leads to a second-order accurate approximation, since in this case the first-order error term

Pressure-corrected SPH with innovative particle regularization algorithms and non-uniform, initial particle distributions

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***Abstract*—This paper will present an enhanced SPH version, including some particle distribution algorithms, for which many of the well-known drawbacks of the standard SPH method are solved or, at least, relieved. Recent innovations in the SPH solver of VPS/PAM-CRASH are discussed in detail. Regularization algorithms to improve the particle distribution, both at the start of, and throughout, the simulation, highlight that such features help to ensure accurate interpolation of relevant fluid properties. A pressure correction method is also discussed. The combined effect of these improvements allows for the artificial viscosity to become small enough to represent the actual shear viscosity. With these modifications viscous drag effects for sinking of objects in water can now be simulated. Periodic boundaries are used to reduce the size of the computational domain and introduction of special damping zones allows to mitigate reflections of free surface waves at rigid boundaries. Application of these features to aircraft ditching will be discussed.**

I. INTRODUTION

Despite the well-known advantages of mesh-less particle methods, general acceptance of smoothed particle hydrodynamics for fluid flow applications in industry is hampered by some of the well-known drawbacks of the 'standard' weakly-compressible WC-SPH method. The drawbacks include generation of irregular particle distributions (clumping and alignment), significant scatter in computed pressures, difficulties in handling some of the flow boundary conditions, and the limitations in defining non-uniform particle distributions. In this paper the options to alleviate these drawbacks will be discussed. In Section II a correction of the SPH density equation will be introduced and be compared to similar published methods. It will be demonstrated that this option yields much smoother results for the computed pressures and that the correction is mandatory to obtain correct results for a typical water entry simulation.

In Section III the general approach to particle regularization and various methods to improve the particle distribution are discussed. Examples for free surface flow will demonstrate that not only the particle distribution may be improved but that also the pressure field becomes smoother. As an additional benefit, there is no longer any need for a high amount of artificial viscosity for some typical flow simulations allowing for the viscosity of water to be included. In Section IV some results will be presented for the generation of non-uniform particle distributions. In Sections V and VI further enhancement of the SPH solver of VPS/PAM-CRASH will be described that allow for more efficient flow simulations in some relevant cases.

The final two sections (VII and VIII) are devoted to two test cases after which some conclusions will be drawn.

II. PRESSURE CORRECTION

One of the outstanding problems of the WC-SPH solution is the rather large variation in pressure, both in time and space. The option of density renormalization (using the Shepard filter) has proven to be one method that allows reducing these variations, in particular for temporal variation, but the remaining variations in space are still quite large. The mass diffusion option proposed by Molteni and Colagrossi [1] provides a significant reduction of these pressure variations. This formulation was later extended with a viscous term and the resulting δ-SPH scheme [2, 3], has been demonstrated to provide superior pressure results.

A slightly different formulation may be obtained by inspection of the time-discretized version of the momentum equations for an inviscid fluid without external forces.

A Simple and Effective Scheme for Dynamic Stabilization of Particle Methods

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***Abstract*—The paper presents a simple and effective scheme for Dynamic Stabilization of particle methods, abbreviated as DS. By performing a set of simple simulations, it is shown that the inappropriateness of the simplified/anti-symmetric pressure gradient models for the Moving Particle Semi-implicid method may cause instability and the unphysical states due to their predominant excessive repulsive forces to adjust the disorder of calculation points. The DS scheme is proposed to resolve these problems with a basis of meticulously adequate repulsive force and shows good reproductions of the main flow features including tensile stress states.**

I. INTRODUTION

The MPS (Moving Particle Semi-implicit) method was originally developed by Koshizuka and Oka [1] for viscous incompressible flow as a Lagrangian mesh-free method. As an advantage, Lagrangian approach brings release of the non-linear advection term causing numerical diffusion. However, a suitable handling of the distribution of calculation points (particles) is necessary to avoid instability and unphysical states. So far, the instability issue in Lagrangian methods has been widely studied beyond the particle methods [2-9]. As for the MPS method, it is reported that the maldistribution of particles is facilitated by either underestimation of interparticle repulsive forces or overestimation of interparticle attractive forces due to relative positions between particles in the process of the pressure gradient term. In particular, the kernel function of the MPS method is designed with a premise of incompressible flow and, as a result, of an expectation of non-overlapping states of particles, therefore, it needs a prudent handling of the glutted attractive force.

Koshizuka et al. [10] modified the original MPS gradient model so that interactions of pressure are defined as purely repulsive forces, excluding attractive forces. This concept is widely followed as a basic model in the MPS method by some so-far proposed modifications i.e. the Corrected MPS method (abbreviated as the CMPS method) [11]. The purely repulsive interaction of pressure is commonly executed by an additional (artificial) force based on the pressure state and the distribution of neighboring particles. Consequently, the strong stability may be obtained in compensation for the loss of the accuracy of the reproduction depending on the pressure states. To stabilize the calculation, an improved deformation of pressure gradient based on repulsive interparticle forces is regularly adopted in the SPH method also. As for an additional term, an artificial stabilizing force was introduced [4] by inserting a stress-dependent term with a constant coefficient.

While, as another approach for stabilization of MPS method, Khayyer and Gotoh [8] proposed a Gradient Correction (GC) scheme to enhance the accuracy as to enable treatment of attractive forces in the pressure gradient term. However, it dose not contain the regulating process for the maldistribution of particles, so that its stability is sensitive to the calculation resolution. It is desirable to introduce a supportive stabilizing force for this problem.

In brief, so-far stabilizing techniques to avoid attractive forces may bring overestimation of repulsive forces. While, another approach to treat the attractive interaction with an accurate evaluation requires the stabilizing repulsive force. In order to obtain faithful interactions including attractive forces together with stability, the least, that is “meticulously adequate”, repulsive force regardless of stress state is required only for the error particles penetrating each other.

The paper highlights the instability and the unphysical states of so-far proposed MPS methods stabilized by repulsive forces or accurate evaluation of attractive forces. A modification, namely a Dynamically Stabilized scheme, is proposed to resolve these problems. The new scheme provides meticulously adequate repulsive forces for both compressive and tensile stress states. It is shown the efficiency in stabilization by adjusting the disorder of calculation points with accuracy for comprehensive MPS applications.

II. NUMERICAL MODEL

In this section, previous MPS gradient terms and their problems are explained. In addition, details of the proposed scheme (Dynamic Stabilization: abbreviated as DS) to resolve the problem is shown. Detailed descriptions of other differential operators of standard and improved MPS methods can be referred to [1], [8], [12].

In MPS method, the gradient operator for the pressure gradient [10] is defined as:

An implicit SPH solution of the Burgers equation.

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***Abstract*—The motivation behind the study of this problem is to go deeper in the understanding of the consistency of SPH methods when applied to problems with increasing levels of difficulty. In [1] and [2], when particles were uniformly placed in the computational domain, the consistency of boundary condition enforcement of Dirichlet and Neumann boundary conditions in 1D and 2D Poisson problems was studied. In the present study, particles move according to the inherent Lagrangian formulation typically found in SPH and consequently, the Laplacian operator and the Poisson solver should be able to obtain a consistent solution for such non-uniform distributions.**

Previous results where non-Lagrangian SPH formulations are applied to 1D and 2D Burgers' problem can be found in [3]. In those cases, SPH is used to transform the differential operators whilst particles are kept fixed in their initial positions. In our case, the complete Lagrangian SPH perspective of the Burgers' problem adds some difficulties to the implementation. The procedure is based on a fully implicit time integration scheme solving a Poisson problem for each time step. The most interesting challenges of this formulation are:

- **Although an implicit formulation is used, the time step must be controlled in such a way that particles do not overpass each other.**
- **The accuracy obtained in the Poisson problem solution is studied, especially with this formulation where the particle distribution is non-uniform.**
- **The non-linear effect creates an accumulation of particles on one of the boundaries of the domain and the accuracy of the solution must be monitored.**

How the distortions, produced by the movement of the particles according to the Burgers equation affect the accuracy and consistency of the problem, is something that must be carefully studied. This work shows a simplified previous step in the absence of a pressure field and the mass conservation equation that are always present in more complete formulations such as the Navier-Stokes equations.

I. Introduction

Different numerical methods have been used for computing the solution of boundary value problems. All these methods have advantages and disadvantages. When a fluid is not confined in a space region, it is usually deformed, and mesh dependant methods such as finite elements, suffer from a lack of accuracy due to severe mesh distortion. This effect could be fixed by re-meshing and interpolating strategies, increasing the complexity of the code and the numerical error due to the interpolation step. Interesting alternatives are of course mesh-less methods such as SPH. Due to the absence of mesh connectivity, this method seems to be ideal for modeling fluid mechanics problems where particle distribution transforms the computational domain even when large deformations are present. However, these methods, see [4], still need some improvements and its consistency compared to mesh dependant methods is still being studied. SPH, [5]–[7], is a classical mesh-free method, invented for the simulation of astrophysical problems. The SPH scheme is a Lagrangian model based on a smoothing of the spatial differential operators of the fluid-dynamics equations and on their subsequent discretization through a finite number of fluid particles. The smoothing procedure is performed at the continuum level using a compact support kernel function whose characteristic length is the smoothing length h. The resolution of the discrete SPH scheme is a function of the smoothing length h and the mean particle distance dx. In this framework, the (continuous) equations of fluid-dynamics should be recovered as both h and dx/h simultaneously tend to zero [7]. Typical partial differential equation problems, are transformed by SPH into an integral formulation. Among the difficulties that are normally found in the SPH methodology, the most studied ones are: boundary conditions, tensile instability, lagrangian deformation and incompresibility condition enforcement. The SPH simulations in engineering usually involve solid boundary conditions (BC) for both the velocity and pressure fields. Generally, two types of boundary conditions are used in SPH: prescribed velocity in a moving or steady wall and constant pressure for a free surface. When the velocity is prescribed in a boundary, a homogeneous Neumann boundary condition is used for the pressure. On the other hand, when a free surface is present, a Dirichlet boundary condition is imposed to obtain a constant pressure on the boundary. These boundary conditions are present in previous ISPH works [8], [9] where the Poisson equation was solved and the pressure was calculated. The methodology used to impose boundary conditions does not differ at all from the ones used by any other discretization methods and in most of these cases, the presence of extra particles is necessary to satisfy the kernel completeness. Another important remark is that very little consistency tests can be found when the discretization parameters (number of particles and the smoothing length) tend to the continuous formulation. In the SPH framework, these conditions have been implemented in the past in a different number of ways: by using boundary forces-type models [10]; by modifying the structure of the kernel in the neighborhood of the boundaries [4]; by creating virtual particles inside the

A Novel Error-Minimizing Scheme to Enhance the Performance of Compressible-Incompressible Multiphase Projection-Based Particle Methods

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***Abstract*—A novel scheme is presented to enhance the performance of projection-based particle methods for simulation of compressible-incompressible multiphase fluid flows. The newly presented scheme is an extended version of a previously proposed one and is developed by considering compressible forms of Poisson Pressure Equation and acoustics. This study also highlights the importance of appropriate selection of error compensating terms and their coefficients in minimizing the projection-related errors. Qualitative and quantitative verifications are made by simulating a Rayleigh-Taylor instability, a violent sloshing flow and a 2D liquid impact.**

I. INTRODUTION

A challenging problem of projection-based particle methods that incorporate a velocity divergence (or density time variation)-based source of Poisson Pressure Equation (PPE) corresponds to accumulation of numerical errors leading to considerable violation of volume conservation. In an attempt to resolve this shortcoming, Kondo and Koshizuka [1] proposed a multi-term source of PPE comprising of a main term and two error compensating terms with constant coefficients for MPS (Moving Particle Semi-implicit [2])-based simulations of incompressible flows. Khayyer and Gotoh [3] pointed out three major shortcomings of this scheme, namely, incorporation of first-order-accurate discretizations, application of constant coefficients, ignorance of free-surface, and proposed a novel ECS (Error Compensating Source) comprising of a high-order main term and two error compensating terms with dynamic coefficients as functions of instantaneous flow field. In the SPH framework, a simplified version of this scheme, hereafter referred to as ECSC, comprising of a main term and an error minimizing term with a Constant coefficient, has been applied [4]. In this paper, we firstly highlight the superiority of ECS, as well as the importance of careful selection of error compensating terms and their coefficients by simulating a Rayleigh-Taylor instability.

The second part of this paper is designated to derivation of a novel ECS scheme for compressible-incompressible multiphase simulations where the effect of relative compressibility becomes important. The new ECS is derived by considering the compressible form of PPE [5] and by meticulously calculating and assigning minimum and maximum theoretical base values in the ECS and thus an allowable range of density variations for the compressible phase. The Compressible-Incompressible ECS is referred to as CIECS. The newly proposed CIECS scheme will be verified by simulating a violent sloshing flow characterized by air entrapment [6] and a liquid impact benchmark test [7].

II. ENHANCED MULTIPHASE MPS METHOD

The basic numerical method applied in this study corresponds to an enhanced multiphase MPS [8] which benefits from five enhanced schemes including the ECS one formulated as follows for incompressible flows:

$$\left(\frac{\Delta t}{\rho}\nabla^2 p_{k+1}\right)_i = \frac{1}{n_0}\left(\frac{\mathrm{D}n}{\mathrm{D}t}\right)_i^* + \left|\left(\frac{n^k - n_0}{n_0}\right)\right|\left[\frac{1}{n_0}\left(\frac{\mathrm{D}n}{\mathrm{D}t}\right)_i^k\right] + \left|\left(\frac{\Delta t}{n_0}\left(\frac{\mathrm{D}n}{\mathrm{D}t}\right)_i^k\right)\right|\left[\frac{1}{\Delta t}\left(\frac{n^k - n_0}{n_0}\right)\right] \quad (1)$$

The first term on the right hand side, i.e. main term, represents the instantaneous time variation of particle number density, while the second and third terms correspond to the instantaneous and accumulative error compensating terms, respectively.

III. A COMPARATIVE STUDY

In this section, the superiority of ECS with respect to ECSC is highlighted by performing a Rayleigh-Taylor instability with a density ratio of 10. **Fig. 1** shows a schematic sketch of this numerical test together with calculation conditions. The ECSC scheme corresponds to that applied by Asai et al. [4] and is formulated as:

$$\left(\frac{\Delta t}{\rho}\nabla^2 p_{k+1}\right)_i = \frac{1}{n_0}\left(\frac{\mathrm{D}n}{\mathrm{D}t}\right)_i^* + \alpha\left[\frac{1}{\Delta t}\left(\frac{n^k - n_0}{n_0}\right)\right] \quad (2)$$

Modelling of Phase Decomposition Using a Fourth–Order Derivation for SPH

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***Abstract*—This paper reports the development and application of an SPH based simulation to the structure forming process of phase decomposition. Phase decomposition and phase separation play important roles in the preparation of precipitation membranes. The methodical motivation is an advantage of the SPH method over mesh-based methods at complex structure changes of the interface.**

We use the thermodynamically–based Cahn–Hilliard equation to calculate phase decomposition. Therefore, the novelty of the present paper is an approximation for fourth–order partial differential equations. The proposed approximation will be applied to binary fluid mixtures with various boundary conditions. The impact of the proposed work will be a stable approximation for fourth–order derivation in SPH.

We compare the accuracy of the presented model with a universal power law for coarsening found by Siggia [1], and observed good agreement. The results for free surface boundary conditions and solid wall boundary conditions will be presented and compared to equilibrium conditions of the system. We conclude that the model allows quantitative simulations for phase decomposition, especially for multi–phase polymer mixtures.

I. Introduction

Phase inversion and phase separation play important roles in the preparation of precipitation membranes. Currently, quantitative prediction is unsatisfactory. Dozens of experiments and simulations have been performed to extend empirical correlations and the understanding of the major aspects of these processes.

Phase separation models based on the Cahn–Hilliard equation [1] describe nucleation and the coarsening dynamics [2] very well. The three consecutive stages of coarsening are diffusion–controlled, viscous–controlled, and inertia–controlled. In the first stage, we use the free energy of a system. Every system tries to minimize its free energy; the strategy is to find a function of the free energy that accurately describes a mixture's physical behavior. Assuming the local free energy depends on the local concentration and the concentration of the immediate environment, Cahn and Hilliard developed a free energy function based on fundamental thermodynamics. They calculated the chemical potential from the variance of the free energy with respect to density. The chemical potential is the driving force in a linear driving force approach.

After the fundamental work of Cahn and Hilliard, several researchers [2]–[10] developed phase inversion models, divided in model B and model H in the classification of Hohenberg and Halperin [11]. Weikard et al. [12] studied the dynamics and the stability of the Cahn-Hilliard equation; Saxena et al., Shang et al. and others [13], [14] compared these results with experimental data. In the 70's, Siggia [15] found a universal growth law for the diffusion-controlled stage.

For the SPH approach, two models for phase separation are developed. Okuzono [5] first studied phase separation for a binary polymer mixture. His approach is similar to the Cahn-Hilliard approach but differs in the main aspect that diffusion of material is not regarded. Okuzono distributed different kinds of particles (e.g. particles of type A and B) and described the separation of the particles by viscous and gravitational forces. Thus, the model only describes viscous-controlled and inertia-controlled phase separation. For the chemical potential, Okuzono used the free energy of the system of Ginzburg-Landau type approximation with an order parameter. Unlike the present approach, Okuzono avoids to calculate the second derivation of the density explicitly; instead, he used the first derivation two times in a row. The Navier-Stokes equation is the transport equation. In the Navier-Stokes equation, Okuzono introduced an additional pressure force as a function of the chemical potential. Additionally, he considered the friction force as a function of the concentration. The results of Okuzono are in good agreement with the power law for coarsening dynamics.

Thieulot et al. [21] developed another phase separation model for a binary mixture. It is based on the GENERIC framework. They derive the chemical potential directly from the entropy of the fluid. It takes the same shape originally suggested by Cahn and Hilliard. Their model is thermodynamically consistent but the effects of diffusive material transport to viscous and inertia forces are neglected.

In this paper, we develop a phase separation model that describes the diffusion–controlled stage using the Cahn-Hilliard equation. It can easily be extended to describe all three stages of coarsening by combination with existing SPH models. As major aspect, we introduce an approach to calculate the fourth–order derivative in SPH.

Most models use periodic boundary conditions. But the effects of boundary conditions on the solution of the Cahn–Hilliard equation are not negligible. Therefore, we discuss different kinds of boundary conditions. Since an extension to multicomponent mixtures is straight forward, we consider only

The SPH Modeling of the Deformation of a Droplet under the Effect of Constant External Electric Field

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***Abstract*—In this paper, the electrohydrodynamics (EHD) forces are implemented into the Smoothed Particle Hydrodynamics (SPH) method. The mathematical formulation of electric forces is presented and transport jump conditions are given. Selecting finite magnitudes of electric permittivity and conductivity of bubble and bulk fluid phases, the leaky dielectric model is used in present work. The results are shown for a quiescent bubble in the bulk fluid and electric forces deform the circular bubble. The direction of deformation elongation depends on the proper selection of electric permittivity and conductivity values of both fluids. Two theoretical solutions are presented and it is shown that the present results are in agreement with these theories.**

I. Introduction

The motion of droplet within a bulk fluid medium takes place in numerous natural and engineering processes such as blood-flow, air entrainment at ocean surfaces, cloud cavitation, boiling heat transfer, petroleum refining, spraying of liquid fuel and paint, and bubble reactors in the chemical industry [1]–[3]. This motion in a viscous liquid is a dynamically complicated, nonlinear, and non-stationary hydrodynamical process, and is usually associated with a significant deformation in the droplet geometry due to the complex interactions among fluid convection, viscosity, gravitational and interfacial forces. Deforming droplet can acquire complex shapes, thereby resulting in a large variety of flow patterns around droplets [1], [4]–[6].

In multiphase systems of different electrical permittivities and conductivities, the utilization of electric fields provides a promising way to control the motion and deformation of droplets which can be crucial for a variety of engineering applications such as electrospray ionization, electro-coalescence and mixing, electrostatic printing and electro-spinning [2], [3], [7]. To state more explicitly, if a droplet suspended in a quiescent viscous liquid is exposed to an externally applied electric field, in addition to the gravitational force induced deformation and motion if exist, it will also be deformed depending on the strength of the applied electric field and the fluid properties such as viscosity, surface tension, electrical conductivity, and permittivity [7]–[9].

Although a number of experimental, theoretical, and numerical studies have addressed the buoyancy-driven motion of a droplet through a quiescent fluid [6], [10]–[12], there are only a few works that consider the effect of the applied electric field on the dynamics of bubble deformation [5], [7], [8], and a complete understanding of the underlying mechanisms has not yet been achieved, which necessitates further studies in this field. Additionally, not only the problem in question but also the large majority of other multiphase flow problems have generally been modeled using mesh dependent techniques [5], [6], [8], [13] and the validity and accuracy of mesh free methods for modeling droplet deformation under the influence of electric field need to be further investigated.

In this study, we investigated the effect of an electric field on the neutrally buoyant droplet in a quiescent Newtonian fluid. The leaky dielectric model is used in order to account for the effects of the electric field, and electrical properties of liquids. In the leaky dielectric model, the droplet with finite electrical conductivity and with no free electrical charge is considered. Under these model assumptions, electric stresses are supported only at the droplet interface, and are absent in the bulk. The interface of the droplet is modeled as a transition zone with a finite-thickness across which the material properties vary smoothly. The surface tension and electric field effects are integrated into momentum balance equations as volumetric forces by using the continuum surface force and the divergence of the Maxwell stress tensor, respectively.

II. Mathematical formulation

A. Mechanical balance law of continua

All constituents of the multiphase system are considered to be viscous, Newtonian and incompressible liquids with constant material properties $D\Gamma/Dt = 0$ where D/Dt is the material time derivative operator, and the arbitrary field Γ may represent the density, and viscosity, among others. The set of equations governing the electrohydrodynamics of viscous fluids is composed of Maxwell's equations, and the conservation of mass and linear momentum which are written in their local form for the volume and the discontinuity surface, respectively as

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\vec{v}, \tag{1}$$

Multi-purpose interfaces for coupling SPH with other solvers

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***Abstract*—An algorithm for coupling SPH with an external solution is presented. The external solution can be either another SPH solution (possibly with different discretization) or a different numerical solver or an analytical solution.**

The interaction between the SPH solver and the external solution is achieved through an interface region. The interface region is defined as a fixed portion of the computational domain that provides a boundary condition for the SPH solver. A ghost fluid, composed by fully lagrangian particles (*i.e.* ghost particles) covering the interface region, is used to impose the boundary condition. The ghost particle evolution, including its position, is integrated in time according to the field of the external solution. The physical quantities of the ghost particles needed in the integration scheme are obtained through an MLS interpolation on the field of the external solution. When a ghost particle crosses the boundary of the interface region, entering in the SPH domain, it evolves according to the SPH governing equation.

The spatial distribution of the ghost particles can become largely non-uniform due to the forcing by the external solution. Thus, a packing algorithm is applied on the ghost particles in the interface region, to guarantee a particle distribution suitable for SPH operators. Since the ghost particles can exit from the interface region, a seeding algorithm is needed to introduce new ghost-particles.

The algorithm is tested on several benchmarks and with the external solutions given by other SPH solvers with different discretizations and by analytical solutions. The technique is deeply investigated in terms of accuracy, efficiency and possible applications. Finally a coupled simulation involving a finite volume solver is presented.

I. Introduction

Meshless methods and, among them, Smoothed Particle Hydrodynamics (SPH) are nowadays well validated options in order to tackle hydrodynamic problems. Some of their features are equivalent to mesh based solvers, and the free surface treatment results easier. One of the most important gaps to bridge is the possibility to use different resolutions in the same calculations. In mesh based methods, techniques as mesh stretching or even multi-block techniques are widely used. This concedes a consequent advantage to calculate boundary layers or more generally in large computational domain. Within the SPH framework, the equivalent to stretching, implemented through a variable-h kernel formulation was introduced by [1] (see also [2]). The kernel size evolves along the domain together with the particle size. The technique is interesting for short simulations where there is no strong mixing, but can lead to stability problems for numerical evolutions over a larger time. A recent achievement is the splitting coalescing scheme presented in [3] following the initial idea of [4] and later study of [5]. Another interesting topic is the coupling of numerical methods, often known as domain decomposition. SPH has been coupled with mechanical model [6], FEM for fluid structure interaction [7], some attempts have also been made to couple with shallow water solution [8].

In the present paper a complete procedure is presented to permit the interfacing of SPH with another numerical solution. It aims to show the capability to divide the numerical domain in subdomains solved by different numerical solvers. This external - from the point of view of the single SPH domain - solution can be either an other SPH calculation or a result obtained with a different technique. This approach theoretically allows full coupling with the external solution and several tests are performed in this goal. Among those the results of the coupling with a finite volume solver are presented.

II. Modeling multi-domain interaction in SPH

The aim of the present work is to provide a full coupling of the SPH solver with an external numerical solver. This means that the solution coming from the external solver has to be used as boundary condition of the SPH solver, and viceversa. The transfer of the external solution to the SPH solver is achieved through an interface region. The interface is defined as a region (area) of the computational domain that provides a boundary condition for the SPH solver imposed by an external solution. The boundary conditions are imposed through the ghost fluid, that is composed by fully lagrangian particles. They cover the whole interface region and evolve according to the field given by the external solution. Then the SPH solution is transferred to the external solver through interpolation of the particle data in a specular manner. The imposition of a generic boundary condition given by an external solver requires the definition and development of specific algorithms that allow for a general representation of the fluid field in the interface region. In the following sections some dedicated procedures are described.

Coupling of a SPH-ALE and a Finite Volume Method

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***Abstract*—This paper presents a novel coupling algorithm of the meshless method Smoothed Particle Hydrodynamics - Arbitrary Lagrange Euler (SPH-ALE) with a meshbased Finite Volume (FV) method. On the one hand SPH is very well adapted for the simulation of highly dynamic flows with moving geometries and/or free surfaces but has difficulties to represent rapidly changing gradients with a constant particle size and a particle refinement is not easy to implement. On the other hand FV methods are well established for fluid simulations but can be tedious with moving geometries and need a special treatment at mesh interfaces, for example between rotating and static parts of the mesh. In order to overcome these shortcomings, we propose a coupling of SPH-ALE with a FV method, where the whole computational domain is covered by SPH particles that can be in Lagrangian motion. FV cells are added in areas where a more accurate (refined) simulation is needed. The coupling is based on a communication in two ways between the domains. FV calculation points are used as SPH neighbors in the overlapping region, while boundary values for the FV cells are obtained by interpolation from the SPH particles, similar to the CHIMERA method of overlapping grids. The approach is carefully validated by means of well-known academic one-dimensional testcases that show encouraging results.**

I. Introduction

The Lagrangian method Smoothed Particle Hydrodynamics (SPH) (see [1], [2]) computes the physical flow fields on a set of unstructured calculation points, called particles, that follow the flow and that have no connectivity between each other. Due to its meshless Lagrangian character the method is very well adapted for flow simulations with moving geometries and/or free surfaces. However, it has difficulties to capture rapidly changing gradients of the flow fields with a constant particle size (see [3]) and particle refinement is not easy to implement because the particles are moving. In addition, the isotropic nature of most SPH formalisms makes it impossible to refine particles in an anisotropic way. Rapidly changing gradients arise for example close to wall boundaries in direction normal to the wall. The common practice in meshbased methods is to refine the mesh mainly in this direction while SPH particles have to be equally refined in all direction, that makes it computational more expensive. Finite Volume (FV) methods are popular meshbased methods that are accurate and stable for many important applications in Computational Fluid Dynamics (CFD). They allow an anisotropic refinement and are well established for the computation of the viscous boundary layer. But in contrast to SPH they necessitate a special treatment at mesh interfaces like between static and rotating parts of the geometry. This rotor-stator interface introduces an additional source of possible errors. Moreover, simulations where geometries are moving in a more complicated way are cumbersome and sometimes even impossible, and the correct detection of a free surface position is computational expensive. The aim of this paper is to combine a meshless SPH-Arbitrary Lagrange Euler (ALE) scheme with a meshbased FV method, in order to combine the best of both approaches. Starting from the same set of continuous equations, discrete SPH equations as well as FV equations can be derived. For the coupling the whole computational domain is covered by SPH particles. In regions of interest, where a more accurate solution is needed, refined FV cells are added, overlapping the SPH particles. In these regions FV calculation points are used as SPH neighbours, while boundary values for the FV domain are interpolated from the SPH particles, similar to the CHIMERA method (see [4], [5]). The CHIMERA method uses one structured main grid and one or several structured grids that are overlapping the main grid for local refinement, e.g. around moving geometries. Boundary values for one grid are interpolated from the others, so that information is correctly transferred. Instead of a structured main grid, we have unstructured SPH particles without connectivity. Therefore, scattered data approximation techniques, like Shepard's interpolation, are employed for the interpolation of the FV boundary values.

II. SPH-ALE

In 1999, Vila [6] introduced SPH-ALE in order to increase accuracy and stability of standard SPH. The starting point is a weak formulation of the Euler equations, written in an arbitrarily moving frame of reference,

$$L_{v_0}(\Phi) + \nabla \cdot F(\Phi, v_0) = Q, \tag{1}$$

with

$$F(\Phi, v_0) = F_E(\Phi) - v_0\Phi, \tag{2}$$

where Φ denotes the vector of the conservative variables, $F_E(\Phi)$ the vector of the Euler fluxes, Q the source term and

On the use of particle based methods for cosmological hydrodynamical simulations

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***Abstract*—In this paper, we attempt to clarify the relation between different particle based methods and try to assess their viability in the context of cosmological simulations. We identify two classes of methods depending on the number of neighbours required to compute a single interaction between a pair of particles. From then, we argue that SPH-ALE is a potential candidate for future astronomy simulation implementations as its computational complexity versus standard SPH does not change. Building on our analysis of the relations between the different schemes, we then attempt to design a novel technique to correct for errors entering the equations of motion of SPH-ALE by using the ALE part of the method and trying to suppress the errors before they affect the flow.**

I. Introduction

Cosmological hydrodynamical simulations are a very active area of research and the number of simulation codes and numerical techniques is constantly growing. Particle based techniques, such as SPH, have been dominating this area thanks to their Lagrangian nature and their ability to naturally track rapidly moving objects. Despite the ever increasing number of particles used in simulations, the resolution achievable by big runs cannot always satisfy the scientific needs motivating such computations. Putting aside the challenging question of the modelling of some astronomical phenomena (e.g. radiative cooling, star formation, black hole accretion, stellar feedback, ...), the difficulty mainly resides in the ever shrinking size of the time steps and the ever growing dynamical range required. To obtain scientifically interesting results, simulations of the formation of galaxies will need to resolve the centre of galaxies, which have a size of a few hundreds of parsecs, while being able to take into account the large scale evolution of the Universe, which impacts scales above 10 mega-parsecs, making the simulations effectively span more than 4 orders of magnitude. These constraints as well as the need for self-gravity force computations are very different from other hydro applications of the SPH method and leads to specific implementations, the most widely use one being the GADGET-2 code [1]. At the same time, cosmological simulations require simple periodic boundary conditions and they don't involve matter-fluid boundaries or free-surface situations. This restricts the problem to the evolution of a perfect gas under gravitational forces, modulo the astronomical effects that will not be discussed here.

The number of particles currently used ($> 10^{10}$) reaches the limits of what is feasible on current computers in terms of memory requirement but also in terms of computing time due to the small time steps imposed by the physics. A run time of more than a month on more than a thousand cores is becoming the standard size. Moreover, these huge simulations make the whole post-processing and analysis increasingly difficult. For this reason, the search for improved schemes, in which the same resolution is achieved with fewer particles, has become an important task. The Voronoï tessellation based code AREPO [2] or the WPMHD code [3] are two recent examples of this quest with astronomical applications in mind.

This paper can be thought of as being a exploration of current schemes to guide decisions regarding future code implementation in the field of cosmology. In the first section, we consider different unstructured numerical methods and evaluate their numerical complexity. This analysis leads us to separate the method in two categories depending on the number of neighbours required per interaction. We then analyse in more depths the relation between the FVPM technique [4] and the SPH-ALE formulation [5]. This allows us to understand the error terms entering the latter formalism and design a potential correction method based on the ALE ability of the method.

II. Unstructured schemes

The requirements of future cosmological simulations broadly presented in the introduction imply that techniques beyond the traditional SPH method have to be considered. It is, however, beyond the scope of this short paper to review all possible hydrodynamics published in the literature. We will consider SPH (for an astronomy oriented review, see [6]) and moving mesh techniques such as the AREPO code

Density diffusion terms and solid wall models in weakly compressible SPH

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***Abstract*—This paper is concerned with the three methods of treating solid wall boundaries in the weakly compressible SPH method. This methods are the boundary force particles of Monaghan and Kajtar [11], the method used by Morris et al. [12] which treats fixed wall particles as real particles, and the method used by Adami et al. [1] which models a solid wall with dummy particles and do not evolve their quantities in time. For each method, we study the effect of the density diffusive terms proposed by [2] on smoothing the pressure field. To compare against realistic exact time-dependent solutions, we simulate the time-dependent, viscous, low Mach number evolution of both axisymmetric spin-down in a cylinder and accelerated fluid in a box.**
These simulations show that all methods satisfy the geometry and kinetics of the flow. However, using several layers of real fluid particles, by evolving their quantities in time, to model the solid wall, gives better pressure distribution than other methods. This method gives the best results when both terms of density diffusion are used and pressure and velocity of boundary particles are interpolated in the way proposed by Adami et al [1].

I. Introduction

Studying turbulence in confined domains has advantages of dealing with more practical and physical problems. For this purpose, it is essential to model the solid walls properly.

Since the first presentation of the SPH method, many formulations have been developed based on this method. Regardless of the application, boundary conditions are still one of the challenging aspects of the SPH method. One of the significant advantages for SPH method is that it simulates free surface flows without any need of using a boundary condition or special treatment for free surface boundaries. Although there are different models to treat the solid boundaries ([1], [4]–[6], [11], [12]) with acceptable accuracies, by our knowledge, there is not still a definite model to satisfy the physically meaningful and quantitatively accurate results for all solid boundary conditions.

In this study, we focus on three solid boundary models because these models are easier to be used in the complex geometries, need less computational efforts, and they have been tested successfully in some specific SPH formulations. The first method is based on the boundary force particles of Monaghan and Kajtar [11] which uses one layer of the boundary force particles. These particles have constant density and velocity and zero pressure and are considered in the momentum and continuity equations of the fluid phase. We refer to this method in this paper as '$boundary\ force\ method$' or 'BF'.

The second one is based on the method used by Morris et al. [12] in which three layers of fluid particles are used as wall particles. The density and the pressure of the boundary particles is evolved in time and they are considered in the continuity and momentum equations of the fluid phase. However, despite the Morris et al.'s method, the velocity of the boundary particles is not affected by the fluid phase and they have their own specified velocity, unless we mention it. We refer to this method in this paper as '$three\ layers\ of\ fluid\ particles$' or 'Morris'.

The third method is based on the method used by Adami et al. [1], here after we refer to this as AHA, which models a solid wall with three layers of dummy particles and do not evolve their quantities in time. We refer to this particles as '$Dummy$' particles. The pressure of a wall particle is interpolated from the pressure of the surrounding fluid particles and the density of the solid particle is computed from the interpolated pressure via the state equation. These pressure and density are used only in the momentum equation. This modification is referred to as '$AHA-p$' in this paper. In this method, also the velocity of the solid particle used in the momentum equation of the fluid phase is interpolated from the velocity of the surrounding fluid particles. Here, we refer to this modification as '$AHA-v$'.

In this paper we study the effect of using diffusion terms in the continuity equation [2], in the combination with each of the solid boundary models, on the flow characteristics. To compare against realistic exact time-dependent solutions, we simulate the time-dependent, viscous, low Mach number evolution of both axisymmetric spin-down in a cylinder and accelerated fluid in a box. The study shows that while all methods satisfy the geometry and kinetics of the flow, a combination of the

SPH hyperviscosity model for incompressible turbulence

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***Abstract*—Simulations of turbulence with SPH is a challenging task. Several turbulence models in a purely Lagrangian framework have been proposed recently [1] [2] [3]. A useful benchmark to test these models is the turbulent energy spectrum unter isotropic homogenous conditions. In [4], we have shown that the standard SPH method is able to recover the correct $E(k)$ in the resolved region (low wavenumber k), but uncontrolled errors due to the post-processing procedure are introduced near the k_{max} region, masking out entirely the physical effects introduced by the adopted turbulent model. Therefore, the improvement of turbulence modeling in a Lagrangian framework relies strongly on our ability to estimate energy spectra up to the maximally resolved wavenumber. In [5], we compare different methods for estimating spectrum and propose a tool that allows us to reproduce it precisely over the entire wavenumber window. Based on this method, the performance of standard SPH to simulate the turbulent flow is analyzed. Furthermore, a SPH-based hyperviscosity model is proposed, which corrects some drawbacks of standard SPH. In particular, simulations of large-scale forced three-dimensional homogeneous isotropic turbulence with hyperviscosity model show that the energy spectrum is in very good agreement with the classical Kolmogorov's theory.**

I. Introduction

Turbulence modeling is the key issue for most computational fluid dynamics simulations. Several turbulence models were developed in the past for grid-based Eulerian methods, but little progress has been made in the context of a Lagrangian framework. Although meshless Lagrangian methods have been developed since more than 30 years, turbulence modeling in a purely Lagrangian framework has been studied only recently. Wagner and Liu have derived multiple scale sub-grid models for Reproducing Kernel Particle Method (RKPM) [6]. In 2004, Shao and Gotoh applied a turbulence model [7] to Moving Particle Semi-implicit method (MPS), a scheme proposed originally by Koshizuka and Oka in [8]. A Lagrangian meshless method for hydrodynamic flow problems which is receiving increasing attention is Smoothed Particle Hydrodynamics (SPH) [9]. Although the early development of SPH is dated back to the 70's, its first application to the study of compressible turbulent flows has been presented by Welton and Pope [10] who in 1997 coupled the scheme with a Monte Carlo/PDF (probability density function) method. In 2002, Monaghan proposed an SPH version of the α-model [11] devised initially by Fobias et al. to describe compressible turbulent flow [12]. In 2003, an interesting LES approach for SPH turbulence modeling has been presented by Pumir and Shraiman [13]. Recently, Violeau and Issa solved a set of SPH-RANS equations based on an eddy viscosity model (EVM) commonly used in classical CFD [1].

Although much effort have been devoted in the past to test the effect of Lagrangian turbulent models in complex free-surface flows situations, few systematic studies have been conducted under isotropic turbulence. A simple but strong benchmark case that allows us to test the accuracy of different turbulent models is provided by the energy spectrum analysis under homogeneous isotropic turbulent flow conditions [4]. Unfortunately, until now accurate results can be obtained only in the low-to-moderate wavenumber range (large scale motion). The drawback lies in the post-processing analysis and it is mainly due to the fact that velocity field defined on a scattered set of data (particle positions) must be interpolated first on a grid, introducing uncontrollable errors specially near the maximal resolved wavenumber. In [5], we have proposed a second-order Moving Least Squares (MLS) scheme as an optimal tool that allows us to reproduce precisely the energy spectrum over the entire wavenumber window.

By applying this method to standard SPH, the energy piling-up or particle thermalization at high wavenumber range is observed in homogenous isotropic turbulence due to the dramatic decrease of its spectral viscosity. A new hyperviscosity model is proposed and applied here to modify the SPH spectral viscosity in order to correct the sub-grid energy transfer in the near-cutoff wavenumber range.

The paper is organized as follows. In section II the basic SPH formulation used in this work is reviewed. In section III, four different numerical approaches to calculate the energy spectrum from irregularly distributed samples will be compared and the most accurate and reliable method for reconstructing the spectra from scattered data is established. In section IV, the performance of standard SPH for simulating incompressible turbulence is studied. The hyperviscosity model for SPH is introduced in section V. Results of our simulation in the case of forced turbulence are presented in section VI where the energy spectrum and PDF of particle's acceleration are studied in detail. Finally, conclusions are given in Sec. VII.

Direct numerical simulation of 3-D turbulent wall bounded flows with SPH

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***Abstract*—The Smoothed Particle Hydrodynamics method with the unified semi-analytical wall boundary conditions is tested in Direct Numerical Simulation (DNS) mode against well established spectral code reference results. In order to achieve this several prerequisites are introduced. This includes a novel method of initializing the kernel wall correction factor in 3-D as well as a limiter for the imposition of a variable driving force based on a fixed volume flux.**

These tools are then applied to a turbulent channel flow with a minimum size. This test case reduces the computational demand while still sustaining turbulence and capturing all the flow physics. The influence of the volume diffusion term on the turbulence is studied in detail, indicating a specific choice for the associated constant. The second, finer resolution, SPH DNS results are in fairly good agreement with the reference spectral simulation DNS results as well as experimental data in terms of first and second moments. Additionally, some preliminary results are presented showing Lagrangian statistics of the DNS.

I. Introduction

Smoothed Particle Hydrodynamics (SPH) has been used to simulate turbulent wall bounded flows for years. However, only a limited number of researchers investigated basic turbulent flows and whether it is possible or not to reproduce their statistical behaviour in SPH. Robinson *et al.* [1] investigated turbulent flows in 2-D, which are significantly different from 3-D turbulent flows [2]. 3-D turbulent flow simulations are scarce due to their significant computational demand. Hu and Adams [3] have recently published a paper investigating decaying and forced isotropic turbulence in 3-D. However, most engineering applications will demand the simulation of turbulent wall bounded flows. Issa [4] performed a 3-D large eddy simulation (LES) of an open channel flow with Reynolds number $Re = 538000$. However, the turbulent intensities did not correspond very well to the experimental values. This can easily be explained by the low resolution which was used in this simulation.

The movement of passive particles in turbulent flows is an issue that crops up in certain engineering applications. This is particularly difficult to simulate with Eulerian methods as interpolation routines need to be used which can significantly influence the result [5]. A Lagrangian method such as SPH would be ideally suited for the simulation of such flows but to the best of the author's knowledge only Hu and Adams [3] have investigated Lagrangian statistics of turbulent flows using SPH. As their simulations used unbounded flows the investigation of Lagrangian statistics in wall bounded flows remains an outstanding issue.

In the present paper our goal is to demonstrate the capabilities of SPH to simulate turbulent wall bounded flows and reproduce the associated statistics both in Eulerian and Lagrangian frameworks. In order to simulate such flows it is essential that the boundary conditions are properly imposed. Ferrand *et al.* [6] show that their boundary conditions can indeed impose both pressure and velocity boundary conditions appropriately both in laminar and turbulent flows. In the remainder of this section a brief description of these boundary conditions is given. This is followed by their extension to three dimensions including a novel algorithm to initialize the kernel correction factor. This is then validated in Section III using two representative simulations. Next, a new forcing term for flows with a fixed volume flux is presented before presenting the main simulations of this paper which show the minimal channel. We will introduce this case in detail and show results of both Eulerian and Lagrangian statistics.

A. Unified semi-analytical boundary conditions

The SPH method used throughout this paper is presented in detail in the papers by Ferrand *et al.* [6] and Mayrhofer *et al.* [7], [8]. In the present section a brief introduction will be given to highlight the main points.

The main difference to the classical SPH methods is that the SPH approximation of a function f is given by

$$[f]_a = \frac{1}{\gamma_a} \sum_{b \in \mathcal{P}} V_b f_b W_{ab}, \tag{1}$$

where $\mathcal{P}$ is the set of all particles, V the volume and W the kernel function which, throughout the paper, is the quintic polynomial by Wendland [9]. Finally, γ is a kernel wall renormalization factor which is defined as

$$\gamma_a = \int_\Omega W(\underline{r}_a - \underline{r}_b) \mathrm{d}r_b, \tag{2}$$

where Ω is the fluid domain. Note that this integral is equal to one inside the fluid domain and only in the vicinity of a

SPH MODELLING OF 3D BODY TRANSPORT IN FREE SURFACE FLOWS

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***Abstract* - A 3D SPH numerical scheme has been developed to model the dynamics of rigid bodies, driven by free surface flows. It is based on the Euler-Newton equations for body dynamics, implemented using the SPH formalism. The scheme has been coupled to a Weakly Compressible SPH model for the main flow.**

The "fluid-body" 2-way coupling terms are modelled through an advanced SPH technique for boundary treatment (Adami et al., 2012), here adapted for free-slip conditions. The "solid-solid" ("body-body" and "body-frontier") 2-way coupling terms are represented using the boundary force particles described in Monaghan (2005). This technique has been modified, in order to model the impingements of entire bodies, even at low velocities.

The resulting numerical model is here validated on a 2D asymmetric wedge fall on still water and a 3D dam break event with transport of a floating body. This last phenomenon has also been experimentally realized during this study. Validation is analyzed by comparisons with measurements, URANS results and theoretical solutions.

I. INTRODUCTION

Body transport in free surface flows interests several application fields: flood events with transport of mobile structures, interaction of surface waves with floating bodies (e.g. buoys, platforms), ice floes, transport of tree trunks or branches in rivers or streams and their interactions with hydraulic constructions, etc..

Several SPH studies have dealt with the transport of solid bodies, driven by free surface or confined flows, mainly in 2D and dealing with single 2-way interactions. They are briefly described in the following.

[17] use the ghost particle method to model a 2D dynamics of a falling wedge into still water. [14] model the interactions between water surface waves and fixed cylinders through the use of the so-called "boundary force particles". Using the same technique, [15] and [16] represent the "fluid-body" interaction terms to model a floating body, driven by surface waves. Adopting this kind of particles, [10] reproduce 2D modular bodies in confined flows. The boundary force particles are still applied in [11], where they also use repulsive forces in order to model "solid-boundary" interactions. [7] represent the transport of 2D bodies in confined visco-elastic flows, deriving a formulation similar to [1] for "fluid-solid" interactions, and repulsive forces, defined for "body-body" impingements. The same authors represent the transport of 2D bodies in confined flows in [8]. [3] model the 3D impact of a falling parallelepiped on still water using a model, which couples Finite Element Method (solid dynamics) with SPH modeling (for fluid particles). Finally [18] directly represent solid-solid interactions by approximating the exact formulation for the collision of two rigid bodies in 3D (using an SPH formalism).

In this context we have developed and validated a 3D SPH scheme for body transport in free surface flows. We have coupled it to an SPH model for the main flow. The formulation of the fluid-body interaction terms is based on an adaptation of the boundary technique of [1], whose original formulation was quantitatively validated on fixed frontiers in 2D. Here we apply a variant of it ([2]), in order to model free-slip conditions. Body-body and body-boundary impingements are represented according to the boundary force particles, as formulated by [12], adapted in [2] to treat whole solid bodies, even at low velocities.

The resulting RSE model has been validated on 2D and 3D reference test cases, where measures and Unsteady Reynolds-Averaged Navier-Stokes (URANS) numerical results and theoretical solutions are available. Finally, the numerical model is validated on a laboratory test case (Basilicata University), a dam break event with 3D body transport, which has been realized during this study.

After this introduction (Sec.I), Sec.II describes the numerical model, Sec.III the main validation tests and Sec.IV the overall conclusions.

II. NUMERICAL MODEL

This section synthetically describes the main features of the numerical model: the balance equations for fluid (A) and body (B) dynamics and then the 2-way interaction terms related to both fluid-body (C) and solid-solid (D) interactions, respectively. Full details are provided in [2].

A. SPH balance equations for fluid dynamics

The numerical scheme for the main flow is based on the semi-analytic approach for boundary treatment ("fluid-boundary" interactions), as described in [4].

According to this approach, the continuity equation takes the following form:

Application of SPH on study of a deep water plunging wave

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Abstract—**Understanding deep water plunging wave is of importance in off-shore engineering. Despite numerous studies in the past, there is still a need for a deeper understanding of the wave breaking process. A laboratory wave experiment [1] has a typical length scale of tens of meters and time scales of a minute while interested features of wave breaking process are of centimeters down to millimeters and of seconds. Challenges arising from an SPH simulation at a laboratory scale are the accurate generation of a desired wave packet, over-loss of wave energy when it propagates over a long distance, particle resolution to resolve the fine details, the two-phase flow. To overcome the challenges, we developed a modeling strategy in which the large scale wave propagation is simulated at coarse resolution domain and the fine scale breaking process is simulated at fine resolution domain nested from the coarse domain. We have done several modifications to the original SPH model [2], including a boundary condition that takes into account velocity and acceleration of a moving boundary (wave paddle), incorporation of a two-phase formulation and code parallelization. Results agree very well with the experiment. Interesting local physics of the wave plunging process that have been observed before but not well explained are revealed. This study also shows potential applications of SPH on studies similar complex phenomena.**

I. INTRODUTION

The breaking of steep surface waves is a common feature in the oceans. It can occur due to the buildup of wave energy from persistent winds or the focusing of wave energies through wave-current interactions, wave-wave interactions, shoaling or interactions with lateral boundaries. It can also occur through the nonlinear evolution of waves leading to instabilities. Depending on the mechanism leading to wave breaking, the breaking process can vary from a relatively mild spilling process characterized by patchy air bubbles near the crest to a strong plunging wave characterized by a plunging jet, air entrapment and violent mixing.

In the past few decades, studies of wave breaking have been carried out intensively both experimentally and numerically, especially the most powerful plunging waves which have most implications on engineering and oceanography. The breaking and post-breaking processes of a plunging wave have been described in several experimental studies. The breaking starts with plunging jet penetrating the front water surface, closing over the air beneath leads to the formation an air tube that rolls forwards and lasts for a very short time before collapses abruptly [3], [4]. The entrapped air tube is soon collapsed with an associated spout of water spray shooting upward near the wave crest [4], [5]. The air tube is eventually broken down into smaller bubbles with larger ones quickly resurface and break [4]. The plunging jet penetrating the front surface also leads to a vertical jet in front of the plunger [3], [5], [6]. Arising from earlier experimental and numerical studies, several key features of wave breaking, including those associated with steep breaking waves, are already well understood. However, the mechanics of the wave plunging process past jet impingement, especially the breakdown of the entrapped air tube and subsequent vertical sprays sometimes observed in the experiments, remains less well understood.

Because of the existence of high nonlinearity at the wave crest, fragmentation of water surface, strong turbulence and the presence of bubbles in the water column, these processes are extremely complex for numerical models, even with Lagrangian methods such as SPH. To capture these phenomena would require very high resolution flow field at the near-field of wave breaking. Moreover, a crucial condition for numerical studies of wave breaking is to model correctly the initial wave form, which often requires a larger scale simulation of wave generation, propagation and focusing of a wave packet. A full laboratory experiment has a typical length scale of tens of meters and time scales of a minute while interested features of wave breaking process are of centimetres down to millimetres and of seconds. The multi-scale nature of the experiment, the fine features to be captured are challenging for an SPH simulation.

For that reason, we developed a modelling strategy in which the large scale wave propagation is simulated at coarser resolution domain and the fine scale breaking process is simulated at finer resolution domain nested from the coarser domain. We have done several modifications to the original SPH model [2], including a boundary condition that takes into account velocity and acceleration of a moving

SPH surface tension model without need for calibration or evaluation of curvature

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***Abstract*—In this paper a novel concept is introduced for the modeling of surface tension. The model is based on discrete (particle) modeling and as such it is not applicable to continuum modeling like conventional CFD. The inter-particle cohesive forces are evaluated in a different way than in other SPH models in the literature. The only model coefficient is the real surface tension coefficient of liquids (water: σ = 0.073 N/m at T = 20° C), which implies that in principle no calibration is needed (i.e. if a certain systematic error is accepted). The model can be applied to weakly compressible as well as incompressible SPH.**

An overview is given of existing SPH surface tension models with their main features. It can be shown that Van der Waals like models do not allow for scaling to other droplet sizes. Existing inter-particle models allow for a limited scaling, but they need extensive calibration. The continuum surface force (CSF) method, as applied to SPH by Morris (2000), is physically correct. However the evaluation of the curvature is computationally expensive and requires calibration. For the reasons above it was aimed for a SPH surface tension model where the evaluation of the curvature is avoided, although its effect must be modeled implicitly, while calibration or fine tuning is limited or preferably not needed.

Our concept for surface tension modeling is explored in case studies. The first case is the validation of stagnant droplets against the Young-Laplace (Y-L) equation. The Y-L pressure is always overestimated, as expected, but the error decreases with increasing number of particles and is acceptable (here within 10%), so that calibration is not needed. The second case is the oscillation of droplets (figure 1), which shows a good agreement with analytical solutions. In both cases the scaling to other droplet sizes is correctly modeled. The third case is the merging of droplets. For this purpose an additional feature was developed to allow for merging, when using the summation density with a volume correction in the density estimate. The fourth case is the break-up of a jet.

I. INTRODUCTION

Surface tension plays an important role in many processes in nature as well as in industrials environments. In the industry there is a wide field of applications, varying from food processing, cosmetics, metal casting to fuel injection systems.

Several surface tension models are available in the SPH literature. A distinction can be made between Van der Waals like models, discrete inter-particle models, and continuum models.

Nugent and Posch (2000) consider the cohesive pressure term in the Van der Waals equation of state. Substitution of this additional pressure results in an extra term in the SPH equation of motion. The resulting attractive force is zero in the bulk fluid, while for boundary particles a force normal to the interface or free surface arises. The model does not require the location of the interface nor the local curvature. Instead a surface tension coefficient is prescribed. To obtain stable and circular droplets, the smoothing length for the attractive force is increased by a factor two. Colagrossi and Landrini (2003) include the cohesive Van der Waals term in the SPH equation of state. Following Nugent and Posch (2000) they include the pressure term in the SPH equation of motion. The model is convenient and for that reason popular. However, it can be shown that Van der Waals like models do not scale with the droplet size.

The Lennard-Jones force describes the short range repulsion and long range attraction between two molecules. The attraction represents surface tension. Monaghan (1994) applies it within SPH as an inter-particle force, to describe the repulsion between fluid and boundary particles.

Tartakovsky and Meakin (2005) model surface tension by inter-particle forces. The force is repulsive at short distances and attractive at large distances. The transitional distance is based on the smoothing length. Kordilla et al. (2011, 2012) propose a similar model, where the surface tension force is modelled as two superimposed forces. The short-range repulsive force and long-range attractive force are evaluated under two kernels with slightly different smoothing lengths. The use of two kernels makes the method more expensive. Due to the smoothing of the surface tension force an extensive calibration is needed. The model allows for a limited scaling with droplet size.

Brackbill et al. (1992) developed the continuum surface force (CSF) method, which treats surface tension as a continuous, 3D effect across the interface. The surface tension force is proportional to the local curvature and applied in a direction normal to the interface. It is popular in CFD, although the evaluation of the curvature is an issue.

Volume reformulation of spatially varying interactions using the example of moving contact lines for a complete surface tension description

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***Abstract*—Some physical interactions do not affect the whole computational domain in the same manner and only occur at specific interfaces, lines or even points in space. Properties like the magnitude of a normal vector, as used in the Continuum Surface Force model (CSF) by Brackbill et al., can be used to determine these specific areas and in the same way can be used as volume reformulation of the locally exerted force. We will show how this idea can be applied to other interactions and that balance equations and volume reformulation can easily be exchanged with the restriction of preserving the integral quantity. With respect to contact lines, Brochardwyart and de Gennes came up with the idea of the "non compensated Young force" as driving force for a moving contact line. The work of Hassanizadeh and Gray is a confirmation to this remaining force as shown in their formulation of the microscale momentum balance equation for a contact line. These fundamentals are combined with the incompressible SPH-scheme of Szewc et. al and the CSF formulation of Morris. The Navier–Stokes equations are solved with an incompressible, predictor–corrector scheme. In this way we are not only able to calculate the equilibrium state of a two–phase interface with a static contact angle, but also for instance able to numerically calculate the evolution of a system into its equilibrium state. This approach can be used to describe many further applications where wetting phenomena play an important role and the dynamic contact angle dominates the system behavior. Together with the capability to model density differences this approach has especially for porous media a high potential to model recent challenges of two–phase transport on the pore–scale.**

I. Introduction

Mass balances and momentum balances are the fundamental equations for modeling phase behavior in a wide range of chemical and mechanical processes. One usually considers bulk phases, and as long as interface phenomena are negligible, volumetric description of the governing equation is straight forward. However, many interesting effects in multi–phase systems just happen at interfaces or even at intersections of interfaces, which are called contact lines. Balance equations can also be formulated for interfaces or contact lines, as Hassanizadeh and Gray [3] showed. If such a condition is incorporated into the governing eqations, one should be aware of the units in this condition. The balance of an interface is written in terms of an area, which has to be transformed into a volumetric description for a complete three–dimensional model. With respect to momentum balances, interfacial conditions must be transformed from a force per area to a force per volume, and in the case of a contact line condition, a transformation from a force per line to a force per volume is necessary.

II. Two–phase model

The Navier-Stokes equations for an incompressible, Newtonian fluid in Lagrangian formulation are given by:

$$\rho\frac{D\vec{v}}{Dt} = -\nabla p + \mu\Delta\vec{v} + \rho\vec{g} \tag{1}$$

$$\frac{1}{\rho}\frac{D\rho}{Dt} = \nabla\cdot\vec{v} = 0, \tag{2}$$

where ρ, p and μ are density, pressure and dynamic viscosity. The vectors $\vec{v}$ and $\vec{g}$ represent velocity and gravitational acceleration. For a complete description of surface tension we extend (1) by two further terms:

$$\rho\frac{D\vec{v}}{Dt} = -\nabla p + \mu\Delta\vec{v} + \rho\vec{g} + \vec{F}^{vol}_{wn} + \vec{F}^{vol}_{wns}. \tag{3}$$

Here $\vec{F}^{vol}_{wn}$ represents the contribution from the interfacial balance equation, which results in the Continuum Surface Force by Brackbill et al. [1]. This force is exerted on the wn–interface, where w denotes the wetting phase and n the non-wetting phase. With the same nomenclature we write the contribution of the momentum balance equation for a contact line as $\vec{F}^{vol}_{wns}$, where the indices wns stand for the contribution of all three phases, see fig. 1 and fig. 2.

A. Continuum Surface Force (CSF)

The Continuum Surface Force for a wn–interface was introduced by Brackbill et al. [1] and the result is first a force per area:

$$\vec{f}_{wn} = \sigma_{wn}\kappa_{wn}\hat{\vec{n}}_{wn}. \tag{4}$$

σ_{wn} denotes the surface tension coefficient, κ_{wn} the curvature of the wn–interface and $\hat{\vec{n}}_{wn}$ its unit normal. The normal is calculated by a weak formulation of

$$\vec{n}_{wn} = \frac{\nabla c}{[c]}. \tag{5}$$

Several approaches to achieve better accuracy of a single precision SPH code

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***Abstract*—Two approaches proposed in this paper allow a developer of a single precision code to get better accuracy for position, velocity and density of particles used in smoothed particle hydrodynamics. The first approach may usually be applied to density and position variables, since their values are changed by a small quantity during time integration. So smaller time steps may lead to relatively large errors in computation used in a single precision code. Therefore we represent these variables as a sum of two ("large" and "small") single precision numbers. The second approach may help to identify those variables which can be representing as functions of other to-be-found variables with better precision. One example of a pair of such variables is density and relative change of density with respect to reference value when density values of particles are within a very small range of a large number. Use of finite number of terms from a corresponding Taylor series and rewriting it in a form of several multiply-add operations may lead to accuracy similar to double precision numbers.**

I. Introduction

Simulation of fluid movement in smoothed particle hydrodynamics (SPH) often requires large number of particles to get good proximity to real life problems. Due to limited size of computer memory a single precision version of an SPH code is often chosen, so a larger number of particles can be modelled. However, this often leads to a reduced accuracy of particles' position, velocity and density and for some benchmarks may produce unacceptable results and various artefacts. So it is very important to decide which variables in a code should have single/double precision. Another technical restriction may arise from computing architectures. For instance graphics processing units (GPUs) are widely used to increase performance of an SPH application, where SIMD (single instruction, multiple data) operations prevail against the other (non-parallelizable) ones. But for cost effective hardware GPU solutions double precision arithmetics may not be fully implemented or have a sufficiently reduced performance. Thus it is very important to develop a single precision SPH code, which may produce accuracy similar to double precision codes. In this paper we will concentrate on ideas allowing us to modify variables and operations in a code rather than changing iterative algorithms used in a simulation.

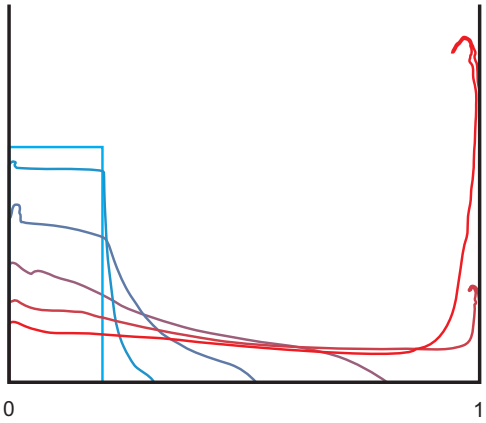

Fig. 1. Two-dimensional dam break (width and height are 1 and 2 for the tank and 0.2 and 0.5 for initial are of water). The water surface is shown for times $t_k = 0.1 \cdot k$, $k = 0, 1, \ldots, 5$.

II. Position Variables

In this section we consider a simple case of two-dimensional dam break. For simplicity all variables used in the paper are dimensionless. There is a tank (the width is 1 and the height is 2) and the fluid (water) has a rectangular shape (the width is 0.2 and the height is 0.5) and is in the left bottom corner of the tank in the beginning of simulation. We simulate position of fluid particles using the standard SPH code (DualSPHysics, version 2) available at [1]. The surface of water for the moments of time $t_k = 0.1 \cdot k$, $k = 0, 1, \ldots, 5$ is shown in Figure 1. One should expect to get the same results independent on the position of the "tank of water" system. Of course, these results depend on number of particles used in a simulation, their masses, speed of sound, smoothing kernels, number of steps used by the iterative solver, etc. However, these results would be identical if computing architectures could use high precision real numbers and arithmetical operations. Unfortunately, finite precision of numbers leads to different results obtained for the system shifted by some vector.

For simplicity we shift the system only along the horizontal axis, i.e. x axis. Suppose the left bottom corner of the tank is at point $(0, 0)$. We call this system a 0-system. A system with its left bottom corner at a point $(L, 0)$ is called an L-

Measures of Particle Disorder

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***Abstract*—In the present work we describe a numerical algorithm which gives a qualitative measure of the disorder in the particle distribution in two dimensions. The proposed measure of the particle disorder has been tested on specific configurations obtained through perturbation of a regular lattice. It turned out that the disorder measure may be qualitatively related to the mean absolute value of the perturbation. Finally, the proposed algorithm has been applied to dynamical test cases characterized by different flow features and by the use of different SPH variants.**

I. Introduction

The attainment and maintenance of a regular particle distribution is a crucial point for all Lagrangian solvers. This is particularly important for SPH schemes because of the smoothing procedure on which these models rely. In fact, a disordered particle distribution implies a drastic reduction of the accuracy of the SPH smoothing operators and may compromise the convergence properties of the scheme itself. Notwithstanding the idea of particle order/disorder is a natural and innate concept, its theoretical definition and quantitative measurement is hard to identify in a clear and unambiguous manner. This is what we try to address in the present work: we propose a measure of the particle disorder in SPH schemes and check it on a number of test cases characterized by different flow features and by the use of different SPH variants.

The basic idea for the particle disorder measure relies on the definition of two different *local* measures (that is, measures associated with each single particle). The first local measure is simply the minimum distance of a particle from its neighbor particles. The definition of the second measure is a bit more complex. For each particle, the kernel domain is divided in four partially overlapping regions. In each region we compute the minimum distance among the neighborhood particles and, then, we take the maximum all over these minimum distances. This procedure is necessary to check any directional anisotropy in the particle distribution. If the distribution is regular, then all the minimum distances coincide and so do the local measures, otherwise, the second local measure is larger than the first one. Specifically, half of the difference between the second and the first measure gives a positive value which is proportional to the relative deviation of the particle from its regular position. The mean of this quantity all over the fluid particles defines the disorder measure.

This global measure has been applied to study specific particle configurations and dynamical test cases. Different SPH variants have been used to understand how much disorder they induce on the particle distribution during the evolution.

II. The particle disorder measure

Let us consider a particle i at the position $\boldsymbol{r}_i$ and define the set of its neighbor particles:

$$\mathscr{N}_i \,=\, \{\, \text{particle } j \neq i \text{ such that } \|\boldsymbol{r}_j - \boldsymbol{r}_i\| \leq R \,\} \tag{1}$$

where R is the kernel radius. Denoting by Δx the initial mean particle distance, we define the first local measure as follows:

$$d_m^{(i)} \,=\, \min_{j\in\mathscr{N}_i} \|\boldsymbol{r}_j - \boldsymbol{r}_i\|\, \Delta x^{-1}\,. \tag{2}$$

Note that $d_m^{(i)}$ is dimensionless. If $\mathscr{N}_i$ is empty, $d_m^{(i)}$ is set equal to zero.

For what concerns the definition of the second local measure, we first divide the kernel domain Ω_i in four partially overlapping regions (see figure 1). In polar coordinates these read:

$$\mathscr{R}_i^{(k)} = \left\{\, (r,\theta) \,\middle|\, r \leq R\,,\, \theta \in [\,(k-1)\pi/2 - \delta\,,\, k\pi/2 + \delta\,]\,\right\}$$

where $k \,=\, 1,\ldots,4$ and 2δ gives the overlapping angle between two adjacent regions. In all the simulations that follow, we set $\delta \,=\, \pi/18\,\text{rad}$. To obtain the second local measure, we first evaluate the minimum distance between the i-th particle and its neighbors in each region and, then, we take the maximum all over these values. Formally, this corresponds to:

$$d_M^{(i)} \,=\, \max_k \left\{ \min_{\boldsymbol{r}_j \in \mathscr{R}_i^{(k)}} \|\boldsymbol{r}_j - \boldsymbol{r}_i\| \right\} \Delta x^{-1}\,. \tag{3}$$

As briefly sketched in figure 1, this definition allows detecting any eventual anisotropy in the particle distribution and, in case of a regular lattice, it coincides with $d_m^{(i)}$. If any region is empty (that is, no neighbor particles are inside it), the minimum distance inside it is set equal to zero. This is done to be consistent with the case in which the particle i has no neighbor particle at all. In this way, the above definitions imply $d_M^{(i)} = d_m^{(i)} = 0$.

Using (2) and (3), we propose a local measure of the particle disorder:

$$\lambda_i \,=\, \frac{d_M^{(i)} \,-\, d_m^{(i)}}{2}\,. \tag{4}$$

By definition, $d_m^{(i)} \,\leq\, d_M^{(i)}$ and, consequently, λ_i is always positive. The coefficient $1/2$ is used to relate λ_i to the relative error between an hypothetical regular distribution and the actual particle distribution (see section II-A). Finally, the global measure of the particle disorder is defined as follows:

$$\Lambda \,=\, \frac{\sum_i \lambda_i}{N}\,, \tag{5}$$

A Switch for Artificial Resistivity and Other Dissipation Terms

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***Abstract*—We describe a new switch to reduce dissipation from artificial resistivity in Smoothed Particle Magnetohydrodynamics simulations. The switch utilises the gradient of the magnetic field to detect shocks, setting $\alpha_B = h|\nabla \mathbf{B}|/|\mathbf{B}|$. This measures the relative degree of discontinuity, and the switch is not dependent on the absolute field strength. We present results comparing the new resistivity switch to the switch of Price & Monaghan (2005), showing that it is more robust in capturing shocks (especially in weak fields), while leading to less overall dissipation. The design of this switch is generalised to create similar switches for artificial viscosity and thermal conduction, with proof of concept tests conducted on a Sod shock tube and Kelvin-Helmholtz instabilities.**

I. Introduction

Artificial resistivity [1] is included in Smoothed Particle Magnetohydrodynamics (SPMHD) [1]–[3] simulations to capture shocks and discontinuities in the magnetic field, similar to the use of artificial viscosity for hydrodynamic shocks. This is accomplished by dissipating the magnetic field about the discontinuity so that the pre- and post-shock states are represented correctly. Similar techniques exist for the treatment of contact discontinuities [4] and interfacial flows [5].

This dissipation is unnecessary away from discontinuities. For astrophysical simulations where high magnetic (and kinetic) Reynold's numbers are common (e.g., $\gtrsim 10^6$ for the interstellar medium), minimising dissipation is critical. Therefore it is important to apply artificial resistivity in a targeted manner, switching on dissipation only near shocks.

Such switches exist for artificial viscosity. The method of Morris and Monaghan [6] use $-\nabla \cdot \mathbf{v}$ as a shock indicator, switching on artificial viscosity in regions of convergent flow. Recently, Cullen and Dehnen [7] have designed a new switch based on using $\mathrm{d}(\nabla \cdot \mathbf{v})/\mathrm{d}t$ as the shock indicator, which they found detects shocks earlier while providing less overall dissipation. Read and Hayfield [8] have a similar switch that uses $\nabla(\nabla \cdot \mathbf{v})$.

A switch for artificial resistivity was suggested by Price and Monaghan [1] (henceforth PM05) analogous to the Morris and Monaghan [6] viscosity switch. However, Price, Tricco, and Bate [9] found even when using this switch, unwanted dissipation was still large enough to suppress the formation of protostellar jets in simulations of star formation. As will be shown in Sec. IV-C, this switch also fails to capture shocks in very weak magnetic fields which would be important in simulations of cosmological and galaxy-scale magnetic fields.

In this paper, we present a new switch [10] for artificial resistivity that robustly detects shocks and discontinuities with less overall dissipation than the PM05 switch. We also generalise the concept to artificial viscosity and thermal conduction. We begin with a general discussion in Sec. II to introduce the equations of SPMHD and the dissipation equations for artificial viscosity, resistivity, and thermal conduction. The new artificial resistivity switch is introduced in Sec. III, with switches of similar design constructed for artificial viscosity (Sec. III-A1) and thermal conduction (Sec. III-A2). Testing of the new switch is performed in Sec. IV, focusing on correctness of shock results, robustness of shock detection, and ability to minimise dissipation. The other dissipation switches are explored in proof of concept tests in Sec. V-A and Sec. V-B. Conclusions are drawn in Sec. VI.

II. Smoothed Particle Magnetohydrodynamics

Ideal magnetohydrodynamics (MHD) is the coupling of the Euler equations with Maxwell's equations of electromagnetism under the assumption of a perfectly conducting fluid (i.e., no Ohmic resistance). This yields the familiar set of Euler equations with a contribution in the momentum equation from the Lorentz force and an induction equation to describe the evolution of the magnetic field.

The SPMHD equations solved are

$$\rho_a = \sum_b m_b W_{ab}(h_a), \qquad h_a = h_{\mathrm{fac}} \left(\frac{m_a}{\rho_a}\right)^{1/n_{\mathrm{dim}}}, \tag{1}$$

$$\frac{\mathrm{d}\mathbf{v}_a}{\mathrm{d}t} = -\sum_b m_b \left[\frac{P_a}{\Omega_a \rho_a^2}\nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2}\nabla_b W_{ab}(h_b)\right] + \sum_b m_b \left[\frac{\mathbf{M}_a}{\Omega_a \rho_a^2}\cdot\nabla_a W_{ab}(h_a) + \frac{\mathbf{M}_b}{\Omega_b \rho_b^2}\cdot\nabla_b W_{ab}(h_b)\right], \tag{2}$$

$$\frac{\mathrm{d}\mathbf{B}_a}{\mathrm{d}t} = -\frac{1}{\Omega_a \rho_a}\sum_b m_b \Big[\mathbf{v}_{ab}\left(\mathbf{B}_a \cdot \nabla_a W_{ab}(h_a)\right) - \mathbf{B}_a\left(\mathbf{v}_{ab}\cdot\nabla_a W_{ab}(h_a)\right)\Big], \tag{3}$$

Accuracy and performance of implicit projection methods for transient viscous flows using SPH

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***Abstract*—Historically, the standard implementation of SPH has relied on the assumption of an artificial compressibility to impose the divergence-free constraint while solving the incompressible Navier-Stokes equations. For viscous flows this simplicity comes at the expense of a stiff timestep constraint coming from acoustic and viscous stability restrictions. Over the last decade, projection methods have been successfully used to satisfy the divergence constraint exactly while removing the numerical contamination often found in articial compressibility methods. We implement a stiffly-stable projection scheme that is second order in time, allowing large timesteps without compromising accuracy. We demonstrate the scheme's superior accuracy and performance compared to weakly compressible SPH and previously employed first order projection methods. Examples of the Taylor-Green vortex problem and flow past an array of periodic cylinders, demonstrate a performance increase of several orders of magnitude when fast algebraic multigrid solvers are used to solve the resulting linear system.**

I. Introduction

In using the Smoothed Particle Hydrodynamics (SPH) formalism to solve for the unsteady Navier-Stokes equations, there have been two main approaches for satisfying the divergence free constraint. In the classical so-called weakly compressible SPH (WCSPH), an artificial equation of state is imposed to obtain a fully explicit method [9]. Originally introduced in a finite-difference context by Chorin [10], the speed of sound introduced by the artificial compressibility provides a penalty term which can be used to control the divergence of the velocity field at the expense of introducing a restrictive timestep constraint based on the acoustic Courant number. This assumption is consistent in the limit of large sound speed or for steady flows. Alternatively, Cummins implemented a projection scheme to solve the divergence free constraint exactly (ISPH), but incur the added expense of solving a Poisson equation at each timestep [11]. In the years since Cummins first introduced the scheme, several investigators have shown that ISPH is able to provide more efficient and accurate answers than WCSPH for steady flows [12]–[16], as ISPH is able to remove the artificial acoustic modes introduced by WCSPH without the need for non-reflecting boundary conditions [17] or artificial acoustic dampening [18].

Outside of the SPH community however, projection methods have been favored over artificial compressibility methods as fast Poisson solvers have become available that allow rapid solution of the resulting linear systems [20]. Further, the unconditional stability properties of these schemes allow the use of large timesteps limited only by the physical Courant number of the problem. By introducing high order projection schemes, it is possible to take these large timesteps without introducing additional error due to temporal discretization. Despite the non-trivial increase in computational complexity of implementing these schemes, combining fast solvers with stiffly stable high order projection schemes ultimately gives more scalable and accurate results than those gained by introducing an artificial compressibility. Further, when investigating low Reynolds number flows, WCSPH suffers from a particularly stiff viscous timestep constraint that can render simulations of large numbers of particles infeasible even in parallel implementations.

It remains unclear however whether standard projection techniques that are typically implemented in an Eulerian configuration can be directly implemented in SPH and whether the techniques used in low order ISPH will carry over to a high order scheme. Projection methods rely on the accurate approximation of discrete Laplacian, divergence, and gradient operators that SPH has been shown to give poor approximations to, particularly for disordered particle configurations [21], [22] While renormalization corrections for the kernel and kernel gradient have been proposed [23] and used successfully in the low order projection method implementations of ISPH, it is necessary to confirm that the operators can be sufficiently resolved to preserve the higher order temporal convergence rates. Additionally, due to the vanishing gradient of the SPH kernel at particle centers, SPH (and particularly ISPH) is prone to a pairing instability [14], [24]. Further, as ISPH enforces a constant density only approximately by fixing a divergence free velocity field, density errors can accumulate, particularly in the vicinity of stagnation points. While a streamline perturbation method [14] has proven effective for removing this instability in ISPH, it remains to be seen whether this success will carry over to higher order projection methods and whether the perturbation will compromise the convergence properties of the scheme. Additionally, in approximating both the pressure and velocity from the same approximation space,

PySPH: A Python framework for SPH

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***Abstract*—We present an open source, object oriented framework for Smoothed Particle Hydrodynamics called PySPH. The framework is written in the high level, Python programming language and is designed to be user friendly, flexible and application agnostic. PySPH supports distributed memory computing using the message passing paradigm and (limited) shared memory like parallel processing on hybrid (CPU + GPU) machines using OpenCL. In this work, we discuss the abstractions for an SPH implementation and the resulting design choices that resulted in the development of PySPH.**

I. Introduction

Smoothed Particle Hydrodynamics (SPH) is a meshless method employing the use of points/particles as discretization entities for the numerical simulation of continuum mechanics problems. The governing PDEs are transformed into ordinary differential equations for particle field variables, constraining individual particles to interact with near neighbors. The subsequent motion of particles with the local material velocity renders the method Lagrangian. This model has been successfully applied to large deformation continuum problems in astrophysics, solid-mechanics and incompressible fluid flow. We refer the interested reader to [1, 2, 3, 4] and the references cited therein for a more detailed exposition on SPH.

The development of SPH algorithms for different problems leads us to the realization that while the applications may be diverse, there exist a fundamental group of operations for any SPH implementation. These include a mechanism to access particle properties, fast neighbor queries to get the interaction lists, discretizations to compute the forces and a time integrator to update the solution. Of these, the force computation represents the "physics", or the particular application area of SPH. Supplementary operations like I/O and post-processing of results are common to numerical simulations by any technique. Fundamental operations notwithstanding, application nuances introduce subtle changes to the algorithm that necessitate a careful design of a general SPH implementation. Further challenges arise when the algorithm is to be implemented in parallel across distributed memory machines and possibly on modern heterogeneous architectures involving hybrid CPUs and Graphics Processing Units (GPUs).

In this work, we describe an open-source, object oriented framework for SPH simulations called PySPH, which is designed to be flexible, user friendly and application agnostic. PySPH arose out of the need for a general purpose SPH tool that hides the implementation details like parallelism from the casual user, yet enables quick prototyping and extension to new problems. With PySPH, the user can choose between solvers for gas-dynamics, solid mechanics and incompressible free surface flows. The solver supports variable smoothing lengths commonly encountered in astrophysical simulations, dynamic and repulsive boundary conditions for free surface flows and multi-stage time integrators. The framework supports distributed memory parallelism using the message passing paradigm (MPI [5]) and limited shared memory like parallelism on GPUs and/or CPUs using OpenCL [6]. While open source, parallel implementations of SPH and particle methods are not new ([7, 8, 9]), users should find PySPH an attractive option to use and possibly extend to their SPH applications. PySPH 0.9beta is released under the BSD license and is publically available at http://pysph.googlecode.com Hereafter, we will drop the PySPH version specification in favor of brevity.

This paper is outlined as follows. Section II explains our motivation behind the development of PySPH by considering an abstract formulation for a continuum problem and the corresponding abstractions required for an SPH implementation. In Section III, we discuss the philosophy adopted in the design of PySPH in light of these abstractions. In Section IV, we provide example results to demonstrate the current capability of PySPH. We conclude this work in Section V with a summary and an outlook to future versions of PySPH.

II. Motivation

Consider the general continuum equations expressing conservation of mass, momentum and energy as

$$\frac{d\rho}{dt} = -\rho\nabla\cdot(\boldsymbol{v}) \tag{1a}$$

$$\frac{dv^i}{dt} = \frac{1}{\rho}\frac{\partial\sigma^{ij}}{\partial x^i} + g^i \tag{1b}$$

$$\frac{de}{dt} = -\frac{P}{\rho}\nabla\cdot(\boldsymbol{v}) \tag{1c}$$

where, $\frac{d}{dt} = \frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla(*)$ is the material derivative, g^i is the component of body force per unit mass and $\sigma^{ij} = -P\delta^{ij} + S^{ij}$ is the stress tensor composed of the deviatoric component S^{ij} and the isotropic pressure P. For solid mechanics, we require a stress model like the Hooke's law, coupling the deviatoric stress to velocity gradients. For compressible problems, an equation of state $P(\rho, e)$ is needed to couple the pressure P to the density ρ and thermal energy e. The equations

Particle refinement and derefinement procedure applied to the Smoothed Particle Hydrodynamics method

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***Abstract*—SPH simulations are usually performed with a uniform particle distribution. New techniques have been recently proposed to enable the use of spatially variable particle distribution, which encouraged the development of automatic adaptivity [6], [14], [21] and particle refinement/derefinement algorithms. All these efforts result in very interesting and promising procedures leading to more efficient and faster SPH simulations. In this article, a family of particle refinement technique is reviewed and a new derefinement technique is proposed and validated through several test cases involving both free-surface and viscous flows. This new procedure allows the user of a SPH code to determine regions of interest where more detailed resolution is needed, based on the technique presented by Feldman [6]. Such technique can be used with several levels of refinement.**

I. Introduction

In Smoothed Particle Hydrodynamics the fluid domain is dicretized using a finite number of particles which represent elementary volumes of fluid. In some cases the size of the fluid domain is very large and therefore to use a constant distribution of particles on the entire domain may become very consuming in terms of CPU and storage. In order to prevent this problem, some authors proposed to use variable particle distribution [1], [8]–[10], [15], [20], [22]–[24]. One of the alternatives is to use a 'variable-h' distribution where the particle interspace is smoothly increased from the region of interest up to the borders of the domain. In these simulations, similar to traditional mesh-based method, the zones of interest with a more concentrated particle distribution are defined as an initial condition. However, due to the Lagrangian feature of SPH, particles can be mixed-up together, so that such approach may lead to strong instabilities. Also, with the 'variable-h' approach the ratio of refinement between one zone to another remains very low (1%)

In order to prevent this problem it is more reasonable to define a dynamic refinement criterion. The first efforts towards adaptive particle refinement in SPH were done for Astrophysical purposes using a density-based criterion to change the particle resolution on regions of interest [11], [12], [18]. More recently, Feldman *et al.* [7] proposed a particle splitting technique where one bigger (mother) particle is projected onto several smaller (daughter) particles. In such a method, the daughter's properties such as mass, volume, density, velocity and pressure are chosen in way that energy is conserved as well as a density continuity is obtained. This technique was a major step towards dynamic adaptivity in SPH as it allows a finer distribution wherever and whenever needed. This technique has already been applied to many problems: from viscous flows [7] to shallow water problems [25]. Later, Lopez *et al.* [14] improved Feldman *et al.* [7] technique by conserving also the density rate of change during the projection procedure, which implied the use of derivative operators.

The efficiency of these refinement algorithms could be enhanced by coupling them with a derefinement technique. Besides the capability of splitting bigger particle into smaller ones, it should be possible to erase then or clump them whenever they are no longer needed. This is not the case of the methods proposed in [7], [14]. Recently, a coalescing technique was proposed by Vacondio *et al.* [26] in which pairs of particles are coalesced into a single larger particle while preserving linear momentum and mass conservation (minimizing the error on density during the process, similarly to Feldman *et al.* [7]).

Here a new particle derefinement technique, simpler than the one presented in [26], based on Feldman *et al.* [7] method and its improved version [14] is proposed. It raises from the assumption that the mother particle can be kept on the simulation instead of being erased and can be advanced in time with the flow. That way, it is possible to switch back to the derefined distribution whenever needed in an straightforward manner as it is shown in this article. The advantage of such technique is its independence of the flow characteristics and the fact that the rate of derefinement is naturally the same as the refinement one. All the details of this new method are discussed in detail throughout this article.

This article is organized as follows. First the governing equations considered are presented together with the SPH formulation. Then the refinement technique ([7], [14]) is detailed followed-up by the description of the new derefine-

A multiscale SPH modeling of near-wall dynamics of leukocytes in flow

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***Abstract*—An efficient multiscale Lagrangian particle solver based on Smoothed Particle Hydrodynamics (SPH) is proposed with application of leukocyte dynamics in large arteries. Based on flow characteristics, the domain is divided into two distinct regions. Due to the high Péclet number associated with hemodynamics in the bulk fluid, leukocytes and red blood cells (RBCs) follow nearly the same pathlines in this region and can be modeled on a continuum basis as transport of passive scalar concentrations. On the other hand, specific particle tracking of the leukocytes is restricted to the near-wall region, where lubrication forces are separately taken into account. Because of large separation of spatio-temporal scales involved in the problem, simulations of RBCs and leukocytes are handled separately. In order to guarantee the consistency of the method, the exchange of leukocytes between the bulk fluid and the near-wall region is taken into account through communication of conserved quantities at the interface between these regions. As the particle tracking is limited to the near-wall region only, our approach brings considerable speed-up to the simulation of leukocyte circulation in large arterial geometries. This has been demonstrated in a test geometry of a backward-facing step which incorporates several flow features observed *in vivo*. Furthermore, the method is easily extended to handle complex three-dimensional patient specific scenarios.**

I. Introduction

Atherosclerosis is the leading cause of morbidity and mortality in the developed world. The disease is characterized by the progressive narrowing and hardening of medium and large arteries. Ultimately this build-up and hardening of material in the arterial wall gives rise to heart attacks and strokes. Sites of atherosclerosis are very focal in nature occurring predominately in regions of disturbed flow, such as the outer walls of bifurcations and downstream of arterial branches. In literature, there are a number of competing hypotheses for site specific atherosclerosis formation. One particular hypothesis is the up regulation of leukocyte intake by the endothelium due to dysfunction; endothelial dysfunction is essentially an imbalance to the regulation of vascular homeostasis [1]. The dysfunctional endothelium leads to over expression of vascular adhesion molecules that bind leukocytes and mononuclear cells to the surface and sub-endothelial space [2], [3]. This adhesion to the surface is thought to be one of the initiating events in the formation of atherosclerosis [4]. Following attachment to the endothelium, monocytes migrate into the sub-endothelial space via inter-endothelial spaces where they differentiate into macrophages (an inflammatory response - that is part of the bodies immune response to fight infection). Within the intima the macrophages release proteins, which recruits further leukocytes into the sub-endothelial space [5], [6]. Hence influx of leukocytes into the arterial could have a critical role in the initiation of atherosclerosis.

Previously in literature a number of studies have considered the transport of leukocytes and other small blood borne particles in arterial geometries related to atherosclerosis [7]–[9] as well as intimal hyperplasia of a distal anastomosis [10], [11]. These studies have highlighted the importance of Lagrangian simulations in studying particle deposition patterns in the initiation and development of atherosclerosis. However it has been also highlighted that the methods used are computationally expensive when considering transient flows in complex geometries. Smoothed Particle Hydrodynamics (SPH) is a popular Lagrangian method that has proven to be capable of handling such problems very suitably. Being originally developed for modeling compressible flow problems in astrophysics [12], [13], SPH applications are extended to a variety of engineering problems [14], [15]. More specifically, SPH has been used by several groups to simulate blood flow and related biological applications [16]–[20].

In the present study we develop an advanced multiscale SPH approach that allows particle methods for hemodynamic simulations to be achieved in a tractable manner. As an example, [11] uses a maximum of 500000 tracers in full domain in a realistic femoral anastomosis geometry to reach convergence. Considering the normal concentration of leukocytes in blood, ca. $10^4/mm^3$, and typical size of large vessels, a fully converged near-wall profile requires computation of trajectories for hundreds of millions of tracers which is about 1000 times more. In contrast, we reduce the number of tracers through specific tracking of leukocytes only in close vicinity of walls. Even though this problem is extremely demanding, our approach brings substantial reduction of computation work.

II. Multiscale particle model

The number of leukocytes in blood is normally much lower than that of red blood cells (less than 1% of whole blood

Shock interactions with dusty gases using multi-phase RSPH

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***Abstract*—In this paper we present results from our newly developed multi-phase RSPH method. We focus on problems related to shock interactions with dusty gases, and discuss the choice of some of the important parameters. Both 1D and 2D simulations are preformed and the results are compared to published experimental and numerical results. The results illustrate the importance of the choice of coefficients, and illustrate the good agreement achieved. For the 2D problem, we study the effect of shock propagation into dusty gases, looking at shock retardation, dust compaction and cloud displacement.**

I. Introduction

A new multi-phase description has been implemented into the Regularized Smoothed Particle Hydrodynamics (RSPH) method. The RSPH formulation takes the work of [1], [2], adapted to applications of shocks and dusty gases, as a starting point. The importance of the different parameters such as drag coefficient and Nusselt number are discussed. Since shock interactions with dusty gases is a challenging topic experimentally, our numerical simulations have been compared both to experimental results where available, as well as to the results from other numerical methods.

II. Choices of parameters

A complete description of the multi-phase RSPH formulation will be presented elsewhere [3]. Here we will restrict the discussion to a few important points. The dust is treated as a separate phase with a separate set of simulation particles carrying information on mass density, velocity, temperature, etc., similar to the way the gas phase is treated. So far we have limited our discussion to the case of dust densities low enough that dust-dust interactions may be neglected. The dust is treated as an inert component, that is, combustion effects are so far not included. In the current work we use spherical dust particles with properties given in Table I. We present results from both 1D and 2D simulations.

The inclusion of dust in the hydrodynamic equations requires the introduction of a number of transport coefficients, such as drag coefficient, Nusselt number and dynamic viscosity. The literature abounds in different empirical expressions for these coefficients, and a more complete discussion could be found in [4]. Here we illustrate the effect by varying one of these coefficients, the drag coefficient, C_d, which we present as a function of Reynolds number in Figure 1. The three different drag formulas illustrate the rather large deviation in the drag coefficient, especially for lower Reynolds numbers. The highest values are found for the Sommerfeld drag [5], the lowest for the Ingebo drag [6]. The choice by Clift [7], is comparable to the Ingebo drag for the lower Reynolds numbers. A more complete comparison of the numerical results obtained for different choices of these coefficient are presented in [3].

The number of experimental studies on shock interactions with dusty gases published in the literature are rather few, but we have compared our numerical studies to the experimental data given in [5]. The Sommerfeld test [5], is a typical shock tube problem, with a shock generated in pure gas, propagating into a dusty gas of homogeneous dust content. Consequently, the dust is assumed already to be in suspension. Based on density data from regular time intervals, the shock position can be determined, as well as the shock Mach number. In the right panel of Figure 1 we have plotted the shock Mach number as a function of position. In the figure, the experimental results [5], plotted with a diamond symbols, are compared with our own numerical RSPH results for the following chosen drag coefficients, [7], [5] and [6], plotted with plus sign, dotted line, and turquoise dashed dotted line, respectively. The somewhat stepwise character for the RSPH results in the figure is due to the averaging method chosen for the data presentation. The numerical results produced with the different drag coefficients illustrate the importance of the proper choice of drag parameter. In comparison with the experimental data, we find the simple Ingebo drag coefficient to give the best fit to the given experimental data,

$$C_D = 27/R_e^{0.84} \qquad \text{for } 6 < R_e < 400. \tag{1}$$

For comparison we have in Figure 1 also included the results of two other numerical methods, presented by [8] and [9]. These show comparable results, although their curves may underestimate the Mach number in the area from $1 < x < 3$ meters. Both these numerical works are preformed with Flux Corrected Transport algorithm using either Finite Element [8] or Finite Difference Method [9].

SWIFT: Fast algorithms for multi-resolution SPH on multi-core architectures

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***Abstract*—This paper describes a novel approach to neighbour-finding in Smoothed Particle Hydrodynamics (SPH) simulations with large dynamic range in smoothing length. This approach is based on hierarchical cell decompositions, sorted interactions, and a task-based formulation. It is shown to be faster than traditional tree-based codes, and to scale better than domain decomposition-based approaches on shared-memory parallel architectures such as multi-cores.**

I. Introduction

Since the past few years, due to the physical limitations on the speed of individual processor cores, instead of getting *faster*, computers are getting *more parallel*. This increase in parallelism comes mainly in the form of *multi-core* computers in which the number cores can be expected to continue growing exponentially, e.g. following Moore's law, much in the same way processor speeds were up until a few years ago.

The predominant paradigm for parallel computing is currently distributed-memory parallelism using MPI (Message Passing Interface) [1], in which large simulations are generally parallelized by means of data decompositions, i.e. by assigning each node or core a portion of the data on which to work. The cores execute the same code in parallel, each on its own part on the data, intermittently exchanging data. The amount of *computation* local to the node is then proportional to the amount of data it contains, e.g. its volume, while the amount of *communication* is proportional to the amount of computation spanning two or more nodes, e.g. its surface. If the number of nodes increases, or smaller problems are considered, the surface-to-volume ratio, i.e. the ratio of communication to computation, grows, and the time spent on communication will increasingly dominate the entire simulation, reducing scaling and parallel efficiency.

Assuming the individual cores do not get any faster, this means that small simulations, for which the maximum degree of parallelism has already been reached, will never become any faster. In order to speed up small simulations, or to continue scaling for large simulations, new approaches on how computations are parallelized need to be considered.

With the above in mind, we will, in the following, describe a reformulation of the underlying algorithms for Smoothed Particle Hydrodynamics (SPH) simulations which uses asynchronous task-based shared-memory parallelism to achieve better parallel scaling and efficiency on multi-core architectures.

II. Algorithms

The interactions in compressible gas dynamics using SPH are computed in two distinct stages that are evaluated separately:

1) *Density* computation: For each particle p_i, loop over all particles p_j within h_i of p_i and compute the particle densities.
2) *Force* computation: For each particle p_i, loop over all particles p_j within $\max\{h_i, h_j\}$ and compute the particle forces.

The identification of these interacting particle pairs incurs the main computational cost, as will be shown in the following sections, and therefore also presents the main challenge in implementing efficient SPH simulations.

A. Tree-based approach

In its simplest formulation, all particles in an SPH simulation have a constant smoothing length h. In such a setup, finding the particles in range of any other particle is similar to Molecular Dynamics simulations, in which all particles interact within a constant cutoff radius, and approaches which

FPM Flow Simulations Using an Adaptive Domain Decomposition Strategy

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***Abstract*—The present paper reports the development of an adaptive domain decomposition strategy to improve the parallel computing performances of our finite particle solver. The domain decomposition is based on a recursive multi-section algorithm, which splits the computational domain into a fix number of subdomains. The adaptive decomposition process changes the size of each subdomain according to its number of particles in order to keep the load constant. The proposed adaptive domain decomposition strategy is validated by a strong scaling analysis of the orbital shaking test case.**

I. Introduction

The Finite Particle Method (FPM) is used to simulate hydraulic applications at high Reynolds number, which involve a complex free surface and moving boundaries. This method is used to improve the consistency of the standard Smoothed Particle Hydrodynamics (SPH) method in the presence of non-uniform particle distribution [1]. However, particle-based methods suffer from a significant increase of computational cost compared to the grid-based methods. To mitigate this drawback, the development of massively parallel codes on multi-CPU or multi-GPU clusters is required [2].

According to Holmes et al. [3] and Basa et al. [4], the use of multi-CPU clusters with an efficient communication allows to reach a near linear speed up. However, a particular attention has to be paid to obtain a uniform load on each CPU. As the computational domain is split in multiple subdomains, and each subdomain is assigned to a single core, the computational time is linked to the most loaded subdomain. Therefore, the size of the subdomains have to be adapted during the simulation [5].

In the literature, two main strategies have been used for the Adaptive Domain Decomposition (ADD) of particle-based methods. The first one is based on the space filling curves, which map the 3D space into a 1D curve. Springel [6] used this strategy in GADGET-2 for cosmological simulations. The second strategy is based on the recursive multi-section algorithm, recently improved by Ishiyama et al. [7].

In the present study, the recursive multi-section algorithm has been used for the domain decomposition. However, the adaptive process is computed by a new approach based on the real subdomain load instead of using the sampling approach from Guibert et al. [8]. The efficiency of the proposed ADD, compared to a fixed uniform domain decomposition, is validated by a strong scaling analysis of the orbital shaking test case. This case study is simulated with the SPH-FPM solver *SPHEROS* developed by Jahanbakhsh et al. [9]. The orbital shaking test case imposes an orbital motion to a cylinder partially filled with water.

In the following sections, we first introduce the neighbor search and parallelization strategy of the numerical code. Then, the proposed adaptive domain decomposition strategy is presented. Finally, the results of the orbital shaking simulations are given and the efficiency of the ADD is discussed.

II. Neighbor search

In the SPH method, each particle has a close interaction with its neighboring particles, which imposes to identify the neighbors of each particle at the beginning of each time-step. However, the basic interacting particle pairs search for N particles has the complexity of $O(N^2)$, which represents a significant computational cost. Hence, more efficient search algorithms, such as Verlet list or octree, are required.

The Verlet list algorithm is usually chosen in SPH codes [10]. In this method, the computational domain is divided uniformly into numbers of subdivisions; see Fig. 1(a). In this case, the distance check is performed for a limited number of particles which are placed in the close-enough subdivisions. This method is very efficient for simple particle systems.

On the other hand, octree search algorithm [6] is able to adapt subdivisions at the location of the particles. Moreover, hierarchy structure of the tree is adopted to suit the needs of adaptive smoothing lengths. With this method, the root octree recursively splits the maximal problem domain into eight octants (Fig. 1(b)). The method is called "complete octree" if the branches at the end of the tree contain individual particle [11]. The Fig. 1(c) displays the 2D complete tree, i.e. quadtree.

To profit both efficiency and adaptivity, one may use the "incomplete octree" structure. In oposition to complete octree, the incomplete octree could have end branches which contain multiple particles. In this case, the branches are split until that the smallest branch length is lower or equal to a specified value.

Integration Of Spring Physics With The SPH Method For Quasi-Solid To Fluid Interaction Using GPGPU Programming

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***Abstract*—Turbines used in an unpredictable natural environment can potentially suffer from the impact of surrounding objects or animals. When turbines are placed underwater this problem primarily comes from large flotsam and substantial marine life. In order to consider the implications of this problem on the design of such turbines it is necessary to be able to simulate numerically a quasi-rigid body and its interaction with rigid boundaries whilst it is suspended in fluid. Smoothed Particle Hydrodynamics (SPH) appears well suited to solving this problem, however methods aimed at simulating elastic bodies and those aimed at simulating fluid flows are typically disparate. Combination of the methods therefore requires a methodology to couple them by way of an interface. Alternatively the SPH methods suited to fluid flow simulation could be combined with a particle based method such as a Mass-Spring-Damper (MSD) model to enforce Hookean restrictions on certain particles within an SPH simulation.**

It is this second possibility which is presented here, where it is shown that the MSD technique neatly combines with a weakly-compressible GPGPU (General Purpose Graphics processing Unit) based implementation of the SPH method. Consideration towards the engineering realism of the elastic body represented by the MSD method is given, with a technique to correct a global spring constant and damping coefficient on a per particle basis presented. Simple extension test cases of a two-dimensional elastic square are provided to highlight the effectiveness of the correction method. Results show good correlation to the expected ideal and questions as to the best method to select a global spring constant are also posed and discussed. An illustrative example of the MSD model inter-operating with the SPH method is also provided.

I. Introduction

A notable problem suffered by fixed turbines placed in a natural environment is that of impact with objects in the surrounding atmosphere. When there is little control over what can come within close proximity of a turbine, the possibility of unintended collision becomes a design consideration.

A recent project [1] to design and implement a system of underwater turbines, with the goal of capturing energy, has led to a need to understand the effects of impact between ocean flotsam and marine animals with such a device. Various issues exist regarding the properties of impact between the rotor blades and potential foreign bodies. The focus of this work is the macroscopic effects of such an impact. Specifically the aim is to provide an overview of the location and magnitude of impact forces as well as considering how they will effect the kinematics of the bodies involved. While the project itself has multiple lines of investigation, some of which are focussed on real-world validation and experimentation, this branch of the project aims to simulate numerically the problem in hand.

Initial investigations need to be based around a simulation technique that can include both moving fixed boundaries (to represent the turbine and rigid flotsam) and potentially highly dynamic fluid mechanics (to represent the surrounding fluid). With this in mind the Smoothed Particle Hydrodynamics (SPH) method has been chosen as its meshless and discrete nature and Lagrangian form allow for violent fluid flows, while its particle-based boundary description intrinsically allows for predefined deformation.

Whilst the SPH method is already well suited to investigation of the effects of impact between rigid flotsam and a turbine surrounded by fluid, the issue of handling the impact of quasi-rigid objects such as a marine animal is less obvious. In this case, the definition of a quasi-rigid object is a three-dimensional volume of varying elastic properties. With this in mind, this paper presents a method of incorporating a Mass-Spring-Damper (MSD) model directly into an existing weakly-compressible SPH software framework. This means that specific SPH fluid particles can be defined as connected by a spring-damper and behave as though they are an elastic object.

The software framework being modified is *DualSPHysics* [2]. This provides a mature and proven implementation of the weakly-compressible SPH method for either CPU or GPU (Graphics Processing Unit) calculation in three dimensions. The latter potentially results in markedly less computation time being required than the former for the same simulation when performed on a workstation. Also provided are pre and post processing tools that allow complex simulation scenarios to be defined.

In order to simulate a quasi-rigid body within a fluid using SPH there are two potential approaches, the first is to couple the weakly-compressible SPH method with a different formulation suited to simulating a highly viscous flow that behaves in a Hookean manner [3], [4]. This was discounted in this instance due to the potential problems of interfacing different SPH methods in an effective multi-phase simulation

AQUAgpusph, a free 3D SPH solver accelerated with OpenCL

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***Abstract*—In this paper AQUAgpusph, a new free SPH software licensed under GPLv3 and accelerated using OpenCL, will be described. Its main differences with respect to other GPU based SPH implementations will be discussed, focusing first on the fact that is accelerated with OpenCL, second on the wide range of solid boundary condition enforcing methods have been implemented (including boundary integrals) and finally on the possibilities that offers its customization via Python scripting.**

I. Motivation

In recent years, numerical computer simulations have suffered an unexpected paradigm change with the introduction of the GPGPU technique, that allows for the use of graphic oriented processing units for more general purposes. These devices have the same computational capabilities than a middle size CPU based cluster for a fraction of the cost, feature that quickly attracted the attention of the researchers in almost every area of science and engineering.

Traditionally, these new paradigm based applications have been developed either in assembly language, or using a graphic implementation specific language, such as GLSL, HLSL or Cg, but with the increasing interest in this technique some manufacturers and researchers have developed high level tools that do more accessible GPU oriented programming to the general public, at which the most famous is probably the CUDA developing language [1], but several many others has been presented too, e.g. BrookGPU, CTM, CBEA or Sh.

Regarding the CPUs, a *technical wall* was reached few years ago due to the impossibility of increasing the processor's clock-rate. The manufacturers dealt with this situation focusing their developments on the multi-core chips with a clock-rate stabilized around 3 GHz. In order to use this new feature, specific new libraries were mandatory, such that most operating systems made their own implementations, although actually the open standard OpenMP [2] is usually applied for all operating systems and architectures.

Therefore a lot of different frameworks exist to develop multi-core parallelized codes, each of them designed for different operating systems or architectures. In order to unify the software development for all these different multi-core alternatives, an open standard has been proposed, the Open Computing Language (OpenCL) [3]. Actually, all major vendors (Nvidia, AMD, IBM, Intel, etc.) have adopted this standard, allowing a unique implementation to be used for massive parallel computations in a wide variety of architectures. The OpenCL features will be discussed later.

Particularly for the Smoothed Particles Hydrodynamics (SPH) method, several implementations have proven the capabilities of graphic oriented devices to perform massive computations using CUDA language [4]–[7].

In this paper AQUAgpusph, a new free SPH software licensed under GPLv3 and accelerated using OpenCL, will be described, focusing on the main differences with other free available implementations [5], [7]–[9], which includes at least:

1) AQUAgpusph is highly modable, 3D, and has been optimised.
2) AQUAgpusph has been accelerated with OpenCL.
3) Most commonly used boundary conditions have been implemented, including boundary integrals [10], [11].
4) AQUAgpusph is Python extensible, which allows to customize and couple solid body motions.
5) Validation tests have been carried out (see e.g. [12] where the boundary integrals method [10], [11] was tested and [13] where SPHERIC benchmark test case number 9 was simulated).

This paper is organized as follows: First, the governing equations of the physical problem that AQUAgpusph is designed to solve approximately are presented. Second, the Weakly Compressible SPH approach implemented in AQUAgpusph is described. Third, the key AQUAgpusph features are discussed, focusing on the differences with other SPH solvers already published. Fourth, A test case is documented, comparing the results with other previous SPH solver, and discussing the performance with 2 different types of computational devices. Finally, a conclusions summary together with future work targets are provided.

II. Governing equations

AQUAgpusph is designed to solve approximately the incompressible Navier-Stokes equations, using for that the weakly-compressible SPH (WCSPH) technique.

Simulating more than 1 billion SPH particles using GPU hardware acceleration

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***Abstract*— The different SPH codes developed within the SPHERIC community are reaching a sophisticated state of maturity in terms of improved formulations and validated calibrations for specific applications. However, one of the main drawbacks of the SPH method is still its high computational cost when real engineering problems must be studied using a huge number of particles. A parallel SPH scheme using heterogeneous clusters of Central Processing Units (CPUs) and Graphics Processing Units (GPUs) has been developed to make the SPH codes more attractive to compete with the other commercial CFD software. The combination of different parallel programming languages is combined to exploit not only one device (CPU or GPU) but also the combination of different machines. Communication among devices uses a Message Passing Interface (MPI) implementation which addresses some of the well-known drawbacks of MPI such as including a dynamic load balancing and overlapping data communications and computation tasks. The paper presents a two-dimensional topology for the domain decomposition which extends the range of problems to which the scheme can be applied. The efficiency and scalability (strong and weak scaling) are analysed for different numbers of particles and different number of GPUs. Last, an application with more than 10^9 particles is presented to show the capability of the code to handle simulations that otherwise require large CPU clusters or supercomputers.**

I. INTRODUCTION

One of the main drawbacks of the SPH method is its high computational cost when real engineering problems are studied, due to the large number of nodal interpolation points, or particles, required for an appropriate description. Therefore, it is imperative to develop parallel implementations of SPH capable of combining the resources of multiple devices and machines allowing simulations of millions of particles at reasonable runtimes. The use of Graphics Processing Units (GPUs) is emerging as a key component in High Performance Computing (HPC) as an affordable option to accelerate SPH with a low economic cost (compared to traditional CPU clusters). GPUs offer now a higher computing power than CPUs. Since the appearance of specific languages such as CUDA [1] that facilitate programming of these devices, many applications with high computational costs are being implemented using this technology and, in many cases, speedups of one to two orders of magnitude have been demonstrated. However, it is important to note that not all applications are suitable for GPU, only those which exhibit a high degree of parallelism. It is no surprise therefore that new computation centres based on GPUs are emerging driven by their computing power and comparatively low energy costs per floating point operation (FLOP). However, the use of a single GPU card is not sufficient for engineering applications that require several million particles that predict the desired physical processes: execution times are high and the available memory space is insufficient. Multiple spatial scales are present in most phenomena involving free-surface waves. Scales ranging from hundreds of meters to centimetres are necessary to describe accurately the coastal hydrodynamics. Thus, most of the relevant phenomena in coastal engineering involve spatial scales over 4 to 5 orders of magnitude. For large simulations it is therefore essential to harness the performance of multiple GPUs.

The present manuscript describes an implementation using a Message Passing Interface (MPI) and Compute Unified Device Architecture (CUDA) to execute SPH. Thus, multi-GPU executions can be performed on heterogeneous clusters where CPUs hosting GPUs are communicated and coordinated. The multi-GPU scheme for SPH simulations presented herein has been implemented in the code DualSPHysics, which is an open-source code available at www.dual.sphysics.org, and is based on the SPH code named SPHysics [2, 3]. The single GPU code has been shown to achieve two orders of magnitude speedups compared to the CPU approaches [4]. Thus, the new MPI implementation was designed starting from an already optimised DualSPHysics code for CPU and GPU [5]. Other previous works to this manuscript described a multi-GPU implementation for the SPH method in [6] and [7] where MPI is used to combine the power of several GPUs hosted in different machines. On the other hand, [8] presented a multi-GPU code but using threads instead of MPI which allows to use a maximum of 6 GPUs hosted on the same machine.

In this paper, the single GPU and multi-GPU implementations are presented while the proposed MPI implementation is described in detail. The results of the multi-GPU approach (improvements and drawbacks) are discussed. Finally, the multi-GPU code DualSPHysics is applied to perform a huge simulation that requires high resolution over a large domain. Thereby, the implementation for SPH method proposed here, enables not only simulations of more than 1 billion particles with a small numbers of GPUs, but also maintains high efficiency when increasing the number of computing devices.

II. PARALLEL IMPLEMENTATIONS

The SPH method can now be executed on a GPU card. All the capabilities of the GPU architecture can be efficiently exploited by using the parallel programming architecture Compute Unified Device Architecture (CUDA) developed by Nvidia. The CUDA implementation in SPH uses threads to perform the tasks by which the particle dynamics are obtained.

The Way to an Enhanced Smoothed Particle Hydrodynamics Formulation Suitable for Machining Process Simulations

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***Abstract*—Setting up a simulation environment suitable to model the process of cutting metal in a realistic way is a rather challenging task. While doing this, a lot of different mechanisms simultaneously influencing the behavior of the considered machining system, e.g. the phenomena of heat conduction and material damage, have to be taken into consideration. Due to several drawbacks of the often used mesh-based methods found for scenarios of the mentioned type, more and more emphasis is placed on the group of meshless simulation techniques in this context. But also the meshless methods in their original formulations do not provide an out-of-the-box solution to the given problem. That is why we present the modifications necessary to acquire an enhanced SPH simulation method that meets the special requirements demanded by the cutting scenario, demonstrate its applicability to the simulation of different standardized test setups and, in a last step, prove the capability of the provided simulation environment to reproduce the behavior of a real processed workpiece observed in experiments.**

I. Introduction

Machining is one of the most important industrial production processes and, therefore, it is of great interest to have a tool suitable to describe the behavior of a real machined workpiece in a simulation. Due to its meshless nature, the SPH method is a quite promising, but frequently not yet known alternative to mesh-based techniques, with the Finite Element Method leading the way, when simulating cutting processes. In order to prove this, we present a broad variety of simulation results generated by our enhanced SPH cutting algorithm implemented in Pasimodo [1], a program package for particle-based simulation methods, including, among others, chip morphology, stress distribution as well as cutting forces, and, furthermore, evaluate them with respect to experimental data. But not only the final results, also the way how to acquire such an enhanced SPH formulation is presented, giving guidance on how to extend the basic SPH code for solids to the equations necessary to model the phenomenon of heat dissipation and the subsequent mechanism of heat conduction in simulations, the purely empirical Johnson-Cook plasticity model along with the related damage model, both taking into account the temperature and strain rate dependence of solid material, and, especially, the ASPH [2] extension presented at SPHERIC 2010. In the context of an ordinary and a notched tensile test, the ASPH algorithm reveals its full benefit when adjusting the smoothing area of each particle in such a way that the unwanted phenomena of a loss of contact between neighboring SPH particles and, thus, numerical fracture are avoided. After having introduced our extended SPH simulation technique, we test the formulation we employ on the basis of an orthogonal cutting process and, this way, demonstrate its capability of simulating the process of cutting metal, in consideration of both mechanical and thermal effects as well as their interdependencies, in a correct manner.

II. Basic SPH Solid Continuum Formulation

The basic equations used to describe the behavior of a solid continuum domain in an SPH simulation are the discretized form of the acceleration equation and the one of the continuity equation given in [3]. In addition to these two relationships, another equation specifying the relation between stress tensor $\boldsymbol{\sigma}$ and the remaining state variables, often referred to as material state equation, is required when simulating solid matter. On the one hand, there is the hydrostatic part of the material state equation, which can be calculated using the Mie-Grüneisen state equation presented in [4]. The deviatoric stress tensor $\boldsymbol{S}$, on the other hand, is determined while, at first, assuming an ideally elastic response of the considered material. Then, in a subsequent operation, the introduced SPH material model is extended to plastic behavior based on the von Mises equivalent stress σ_{vM}. With the von Mises stress and the yield strength σ_{y}, a plastic character of the material is identified in the case that the von Mises yield criterion

$$f_{\mathrm{pl}} = \frac{\sigma_{\mathrm{y}}}{\sigma_{\mathrm{vM}}} < 1 \tag{1}$$

is met. If f_{pl} shows a value lower than 1, the stress state found for the elastically calculated deviatoric stress tensor $\boldsymbol{S}_{\mathrm{el}}$ is located outside the von Mises yield surface and, as a consequence of this, that part of the stress tensor $\boldsymbol{\sigma}$ being responsible for the plastification of the material is reduced following the relation

$$\boldsymbol{S}_{\mathrm{pl}} = f_{\mathrm{pl}}\, \boldsymbol{S}_{\mathrm{el}} \tag{2}$$

in order to bring it back onto the given yield surface.

Shock loading of layered materials with SPH

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***Abstract* — Hypervelocity impacts into structures produce shock waves propagating through the colliding bodies. SPH has given insight into shock loading of homogeneous materials; nevertheless, shock wave propagation through solids with discontinuous density distribution, has not been considered in depth, yet. In previous studies using SPH, impact loading of laminated or composite materials was modeled by homogenization of the structure or under the assumption of being functionally graded materials. Both models neglect the reflection-transmission effects on the interface of different density materials. To capture these reflection-transmission effects, a holistic treatment for the multi-phase material is proposed, with kernel interaction over all parts of the structure. The algorithm employs a variable smoothing length formulation. A dissipative mass flux term is also introduced in order to remove spurious post-shock oscillations on the interface of different materials. In this paper, the SPH solution is presented, along with a relevant benchmark case. The algorithm's performance is studied and the necessity of a variable smoothing length formulation is investigated.**

I. INTRODUTION

The shields of spacecraft in orbit experience impacts by small sized particles of space debris which travel at speeds of 10km/s. These Hypervelocity Impacts (HVIs) are characterized by the projectile's velocity being higher than the target's material speed of sound. Sharp density changes occur, propagated through the target as shock waves. Normal stress effects on an incremental element of the material overweight the deviatory stress effects and hydrodynamic loading regime occurs [1, 2]. Solid materials will effectively behave like fluids in this loading regime. HVIs are typical processes involving extreme compressibility effects of solids, making them substantially different than ballistic impacts.

The efficiency of Smoothed Particle Hydrodynamics (SPH) in simulating HVIs was exhibited in the original simulation of HVI events into monolithic materials by Libersky et al. [3]. Later combined numerical and experimental works established the method as the state-of-the-art tool for HVI simulations [4,5]. Within SPH's context, disintegration of materials under impact is described without severe algorithmic complexity, compared to other methods like Finite Elements Method (FEM) [2].

Shields of multi-material structures have a lower weight-to-performance ratio and are preferred to monolithic ones [6]. SPH was also used to simulate HVIs into multi-component structures [7-9]. Johnson et al. [10] suggested a special interface algorithm to treat non-bonded interfaces (e.g. projectile/target), claiming that when two bodies exchange momentum through simple SPH kernel interaction large errors are produced; this observation was also studied by Campbell et al. [11]. Homogenized materials were introduced in [7-9], with properties the averaged properties of their components. A rigorous procedure of producing averaged versions of anisotropic materials [2,7-9]. Nevertheless, two major drawbacks are apparent in this approach: the homogenization process is based on assumptions coming from quasi-static loading regimes, and the effects of shock reflection-transmission are neglected.

In the case of layered composite materials, shock waves will not propagate undisturbed through the specimen. The transition from one layer to its adjacent layer is not a smooth function of space; it shows up as a discontinuity in the density distribution of the target and reflections-transmissions will occur, whenever a shock encounters a material interface [12]. Hence, the shock loading problem becomes a multiphase shock problem.

SPH algorithms for multi-phase simulations focus on incompressible flow regimes [13-15]. In another approach, the Modified-SPH method is introduced [16] to solve an elastic wave propagation problem through a functionally graded material. The properties of such a material are smooth functions of space. Therefore, without any discontinuities in the properties of the material it is impossible for any transmission-reflection pattern to occur.

The type of artificial viscosity introduced by Monaghan and Ginold [17] is used in all previously mentioned studies. It is a popular way to remove the spurious oscillations in the vicinity of the shocks. An alternative shock capturing technique is the implementation of a Riemann solver in the SPH scheme; such SPH algorithms are described by Intuska [18] and Cha et al. [19]. In a similar manner, an SPH scheme based on the acoustic approximation of the Riemann problem is developed by Parshikov et al. [20].

SPH Simulations of Abrasive Processes at a Microscopic Scale

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***Abstract*—We present the development of smoothed particle hydrodynamics (SPH) simulations for the investigation of the industrial application of abrasive flow machining (AFM). This process cannot be observed in-situ in experiments and therefore demands for numerical simulations at a grain-size process scale.**

There are only a few numerical models available for the AFM process, which are strongly simplified. In order to optimize the machining, an explicit approach of including individual grains in the abrasive suspension is essential. These grains are simulated by individual clusters of SPH particles, which are integrated in time by a rigid body solver.

For the correct force transmission between the suspended abrasive particle and the workpiece, a realistic representation of the stress in the fluid model of the suspension is necessary. Therefore, the rheology of the fluids, containing the abrasive grains, has been experimentally characterized. Since the tested suspensions show a viscoelastic behavior, we have employed a viscoelastic fluid model and have used experimentally gathered data for the calibration of the applied numerical model. The abrasive process on a workpiece and the removal of material from its surface is modeled by the Johnson-Cook ductile flow stress model in combination with a strain-based failure criterion.

We show that the particle method can reproduce key aspects for the simulation of the process of abrasive flow machining. By the application of the Johnson-Cook model, we are able to determine wear contacts between solid materials on a microscopic scale.

I. Introduction

Abrasive flow machining (AFM) is a widely applied industrial manufacturing technique for technical materials and components, which rely on the precise finishing of surfaces in order to achieve their designated performance. It is usually applied for technical components exhibiting complex geometries. However, obtaining the necessary surface roughness and a sufficiently high material removal rate in the finishing process of hard-to-access surfaces remains a great challenge. The abrasive process itself consists of cutting, burring, and surface polishing at a microscopic level. The complex interaction at the wear contact between the fluid, the abrasive particle, and the technical component cause great difficulties in optimizing the process parameters for satisfying results.

The AFM process is usually applied for the finishing of complex internal geometries. Depending on the geometrical size of the inlet and the internal structure, fluids of different viscosities are applied. For inlets and structures with a small cross section fluids of low viscosity are used, while for larger geometries highly viscous and viscoelastic polymeric fluid media are applied. Together with the embedded abrasive grains, this suspension is forced to flow along the internal contours of a technical component. The relative motion of the abrasive medium and the workpiece at contact then causes the wear of material. The aim of optimizing the process parameters for a given workpiece in industrial applications is usually only achieved by trial-and-error. The difficulties to adjust the parameters correctly for a cost efficient finishing of each technical component prevents its utilization in a greater variety of industrial applications despite its huge range of application.

Numerical investigations possess a great possibility to study the process of AFM at a microscopic level. However, there are only a few physical models available and the applied models are strongly simplified, e.g., abrasive grains are considered to be homogeneous, therefore neglecting their individual structure. Until now, there are no numerical simulations available that take into account the individual grain characteristics and their highly dynamic interactions with the workpiece and the fluid at the instant of the wear contact. However, in order to optimize the wear of the material, an explicit approach of including individual particles in the abrasive suspension is promising.

The long term goal of this work is to study numerically the process of abrasive flow machining at a scale where the actual interaction between the abrasive grain and the technical component occurs. Knowing the interaction at the grain size scale, we intend to develop analytical models for the removal rate at the length-scale of the workpiece. This would allow to derive process parameters and to design suspensions with specific abrasive characteristics for a given industrial application. Our goal is to develop numerical tools and models that include the precise coupling between various viscous and viscoelastic polymeric suspensions, the abrasive grains and the technical component.

In section II, we will shortly review the underlying physical models and the SPH framework applied in our numerical approach. Section II-A introduces the concept of viscoelastic media and their numerical approximation. Plasticity models and a fatigue failure criterion is discussed in section II-B. Section III compares the numerical methods to analytical or experimentally gathered data. A short example of a simulation

SPH modelling of the flow field with spilling generated by a hydrofoil

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***Abstract*—This paper shows the results of the SPH modelling of the spilling-type breaking flow field produced by a NACA 0024 hydrofoil positioned in a uniform current, based on the laboratory experiments by Mossa (2008). Understanding wave breaking is fundamental for many coastal engineering problems. It is well known that turbulence and undertow currents in the breaking zone are key factors in the mixing and transport processes. Experimental investigations were carried out by measuring the velocity field with a backscatter, two-component four-beam optic-fiber LDA system. SPH simulations were obtained by a pseudo-compressible XSPH scheme with pressure smoothing; an algebraic mixing-length model and a two-equation model were used to represent turbulent stresses.**

The study made particular reference to the velocity and free surface profile with the aim of analyzing the hydraulic jump development downstream of the hydrofoil. The agreement between the numerical results and laboratory measurements in the wake region is satisfactory and allows the evaluation of the wave breaking efficiency of the device by a detailed analysis of the simulated flow field.

I. INTRODUTION

In the present study, a comparison between 2D SPH solutions and experimental Laser Doppler Anemometer (LDA) results on the spilling type breaking generated by a hydrofoil in a free surface current is shown. Experimental studies on breaking waves are particularly difficult to carry out. Spilling type breaking flows can be those generated by wind waves (known as white caps), in contrast with plunging type breaking. In the spilling type breaking category, Tulin and Cointe [1] showed a distinction between spilling type breaking in shallow water (bore) and spilling type breaking in deep water. In order to better analyze the flow, Battjes and Sakai [2] used a hydrofoil, observing that this solution enables simulation of a sea spilling type breaking.

Following the results by [3], the present paper intends to investigate the adequacy of different turbulence models in representing the flow by comparing 2D SPH solutions of the spilling type breaking flow field produced by a NACA 0024 hydrofoil positioned in a uniform current, with water elevations and velocity profiles measured at several flow sections downstream of the hydrofoil [4].

II. EXPERIMENTAL SET UP

Experimental investigations were carried out in the hydraulic laboratory of the Water Engineering and Chemistry Department of the Bari Technical University, Italy, in the 0.40 m wide, 24.4 m long Plexiglas channel shown in Figure 1, which has a sidewall height of 0.5 m.

Discharges were measured by a triangular sharp-crested weir. Measurements of the upstream and downstream water depths were carried out with electric hydrometer-type point gauges, supplied with electronic integrators which allowed estimation of the time-averaged flow depth. The hydrometers were supplied with verniers allowing us to obtain a measurement accuracy of ±0.1 mm. Water discharge and hydrodynamic conditions were regulated by two gates placed at the upstream and downstream ends of the channel.

The velocity field was measured by using a backscattered, two-component, four-beam fiber-optic LDA system. A 5W watercooled argon-ion laser, a transmitter, a 85 mm probe (having a focal length of 310 mm and a beam spacing of 60 mm) and a Dantec 58N40FVA enhanced signal processor were used. The laser wave lengths were 488.0 nm and 514.5 nm.

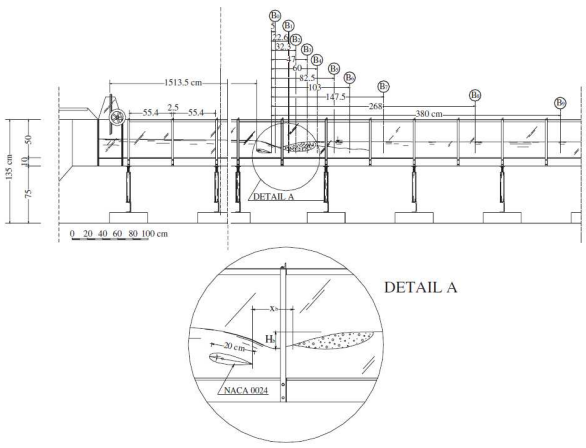

Figure 1. Sketch of the experimental set-up and sections where LDA measurements were obtained.

Slam Modelling with SPH: The Importance of Air

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***Abstract*—The slamming of a solid body into water is a complex and important process with many real-world applications. First investigated theoretically by von Karman in 1929, interest in the topic has been reignited in recent years, given the desire to improve the efficiency and survivability of bed-mounted and floating off-shore renewable energy devices. Motivated by experimental investigations (undertaken at the University of Manchester) of a horizontal metal plate slamming into a wave crest and flat water surface, in this paper the application of SPH to slamming is investigated. The problem is, in general, multiphase: air, either entrained in the water or trapped above the surface, plays a crucial role in dynamics as it acts to cushion the impact. As the velocities in the air phase in the moments before impact can be comparable to the speed of sound, the novel multiphase incompressible-compressible SPH method (ICSPH) [1] is used to model the two-phase water-air system. Comparisons are made between ICSPH, single-phase ISPH, and experimental results. The agreement between the ICSPH and experimental results is very favourable - emphasising the importance of the air phase, particularly for flat surface slam. ICSPH predictions include greatly reduced impact pressures, and deformations and jet formation at the water surface in the moments before impact.**

I. Introduction

Slam loads on offshore structures due to waves are of great practical importance. For example, slam on the underside of platform decks has become more prominent with the bed subsidence associated with oil and gas extraction from below the sea bed. Furthermore, structures are now being deployed to support wind turbines in coastal waters and provide substations for connection to the electricity grid; here slam loading is another important design consideration. The impact loads due to slam on the underside of high-speed craft and during aircraft ditching are equivalent hydrodynamic problems. The magnitude of the almost impulsive impact pressure is particularly uncertain and difficult to predict. Impacts are often associated with loud bangs - indicating that the air phase may be significant.

Von Karman [2] made some of the first theoretical insights into slamming for application to seaplane landing; assuming incompressible, inviscid flow and neglecting gravity, he considered a circular cylinder to be an expanding flat plate with the water surface remaining flat. Wagner [3] extended this to the 2D wedge entry problem including local analysis of jet structures. The case of a flat plate hitting still water has since been studied experimentally by a number of authors over several decades (e.g. [4]–[7]). A more recent study by [8] categorises the impacts observed from their experiments on free falling plates at small impact angles. For very small impact angles they note smooth impact pressure distributions due to the cushioning effect of trapped air. For angles greater than 4°, they observe "Wagner-type" impacts characterised by very large, sharp pressure peaks. Huera-Huarte et al. [9] have undertaken experimental investigations into the slamming forces on flat sandwich panels impacting a free surface at a variety of impact speeds and angles. A good agreement with asymptotic theory, e.g. [10], was found for large impact angles, but, at small angles, the theory considerably overestimated the loading forces due to the increasing influence of trapped air.

The role of air in the slamming process is thus thought to be important in determining the pressure and local forces generated at impact. Experimental findings (e.g. [8]) generally agree that trapped air helps to cushion the impact and reduce impact pressures. In the case when air is not trapped at the surface but entrained in the water, a theoretical analysis by Peregrine and Thais [11] indicates that impact pressures can be reduced by an order of magnitude. However in numerical investigations, the influence of the air phase is often neglected. As pointed out in Oger et al. [12], this produces disagreement with experimental results in the early stages of impact and it is in these early stages that the most violent and potentially damaging peak pressures occur.

In recent years, Smoothed Particle Hydrodynamics (SPH) has shown a great deal of promise over other, more traditional, numerical methods in its ability to model highly deforming, violent free-surface flows. Given the relevance of such flows to many slam problems, SPH has been utilised by a number of investigators to gain further insights into slam processes. Gao et al. [13] investigate wave slam onto the underside of a deck using a Riemann-enhanced single-phase SPH formulation. Their predictions for the impact pressures on the deck are in reasonable quantitative agreement with experiment. Oger et al. [12] undertake a numerical study of wedge-entry problems using a variable smoothing length SPH method. Their results are in good agreement with experimental and analytical results for a number of important measures, including accelerations and pressures. However, they note the greatest discrepancies with experiment occur at the very start of the impact as air cushion effects are not modelled in their formulation. Shao

Comparison of SPH and VOF simulations with experimental measured wave-induced impact loads due to Green Water Events

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***Abstract*—Green water (water-on-deck) and subsequent wave impact is a strongly non-linear, random and complex phenomenon that represents a danger for moored vessels and for vessels in transit.**

The increased use of floating production, storage and offloading units (FPSO) for offshore oil production in areas prone to green water events has heightened the industry's focus on wave-induced impact loads as an important design parameter.

The main focus of this paper is to investigate the potential for using the Smoothed particle hydrodynamics (SPH) method for green water problem by comparing with the commercial CFD tool Star-CCM+ based on its Reynolds Averaged Navier-Stokes Solver (RANS) and the Volume of Fluid (VOF) method and by validating against model test experiment [1]. We have previously presented an approach for modeling green water events using SPH based on a complex velocity inlet boundary condition where we focused only on the kinematics of the water on deck [2]. This complex velocity inlet boundary condition makes it possible to use identical inlet boundary condition for both SPH and VOF methods. The "Kinema3" tool is used to generate these spatio-temporal inlet conditions. The "Kinema3" tool allows us to use the real model time series of incoming waves. This enables the direct comparison of the Green water simulation with experiments. We use the fixed ghost particle method [3] to represent the solid wall condition in our SPH calculation.

For industrial use the calculation time and the simplicity of the simulation setup are important criteria which are also analyzed in this paper.

I. Introduction

Nowadays enormous development of High Performance Computing (HPC) makes it possible to reproduce a strongly non-linear, random and complex events observed during model tests such as breaking wave impact on structure using the classical Computational fluid dynamics (CFD) method RANS-VOF [4]. This can be interesting from an academic point of view but the offshore industry cannot directly use this technique.

This is due to the sensitive nature of this kind of events. It is known that several repetitions of the same slamming event in the model tests can result in a range of slamming forces varying with an order of magnitude [5]. Thus, one can only deal with such phenomena in terms of extreme value statistics. The generation of enough events is still not possible numerically using any CFD techniques. It is also not possible to always perform enough model tests to observe an adequate number of events for good statistics. Therefore, Marintek has developed simple, robust and fast methods in the last decade ([6], [7] and [8]). These methods (WaveLand [6], Kinema2 [8]) and the newly developed Kinema3 are able to generate a high number of three hours simulation in order to identify green water events and in order to build a good statistical basis for the extreme value statistics. These programs still work best with model test data together because it is necessary to use some empirical factors.

The model test observations [9] suggest that the vessel motion can effectively be simulated based on the prediction of the linearized potential theory panel method such as the commercial potential theory panel software WAMIT. This is not true for the estimation of the diffracted waves near the vessel. A combination of nonlinear wave kinematics with the linear ship-induced wave diffraction calculations (defined by the above mentioned panel method), and with empirical factors (such as the wave height factor and the wave velocity factor) can give satisfactory results. Knowing the vessel motion and the diffracted wave height at the hull makes it possible to estimate the relative wave elevation and the water particle velocity at bulwark locations. Usually, one is not interested in the number of the green water events but the hydrodynamic loads during these events. The relative wave height, i.e. height of the water column over the deck and the estimated water velocity can be used to evaluate analytically the water propagation on deck and the slamming loads on vertical structure on deck [8] with the classical hydraulic theory [10]. This method is accurate and robust enough as a simplified tool for engineering design analysis purposes. It has its shortcomings to handle complex geometry on the deck and to predict the load time history.

We have previously presented an approach for modeling green water events using SPH based on a complex velocity inlet boundary condition where we focused only on the kinematics of the water on deck [2]. The "Kinema3" tool allows us to use the real model time series of incoming waves at the location of the vessel. This enables the direct comparison of the Green water simulation with experiments. In this paper, the event with the largest measured slamming force is chosen for comparison. Kinema3 simulation in the time domain is validated against the measured relative wave elevation and

Simulation of extreme waves impacts on a FLNG

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The offshore exploration in severe environments requires mastering the design of ships in extreme conditions. The knowledge of the hydrodynamics impacts is therefore crucial to limit the risks and to optimize the design of ships. The SPH method is particularly well suited for applications involving hydrodynamics impacts with complex geometries, fast dynamics and free surface flows. The objective of this paper is to demonstrate that the SPH method is an efficient method for this type of application. To this end, this paper reports application of the SPH method for structure under extreme sea (greenwater). Comparisons with experimental results are provided.

I. INTRODUCTION

During storms and severe sea states, damages suffered by ships or offshore structures can be particularly important, possibly putting human lifes in danger, destroying equipment on board, or leading to environmental pollution. Examples of such events regularly occur and the offshore industry, as well as engineering teams and classification societies are fully aware of the need in improving the evaluation of extreme loads. These extreme loads cover a wide range of events, like the violent impact of a wave onto the ship hull –slamming impact-, the water flooding of ship decks, blowing away all the equipment –greenwater phenomenon-, or the sloshing inside the oil tanks.

Such events on ships result from an interaction between a wave train and a structure. From a numerical point of view, one has to solve two different kinds of problem with very different typical spatial lengths and time durations. It involves wave generation and propagation onto the structure, with highly nonlinear waves, irregular sea states, whose typical length and duration are respectively 300m and 10s. Eventually, the interaction between the liquid and the structure leads to impacts, with typical length and duration 5 orders smaller (1mm and 1ms). Moreover, some compressibility effects could occur in the gas, and even in the liquid during impact. Hydroelasticity (deformation of the structure under the fluid loads) should also be addressed. The full problem involves a lot of physics, and the present paper is a first step towards the simulation of all phenomena occurring during impact.

Regarding the impact simulation, special attention has been paid to the Smoothed Particle Hydrodynamics (SPH) method. Indeed, the SPH method offers advantages over classical numerical methods when simulating impact type problems. No connectivity is required for the free surface, enabling the simulation of violent flows with possible fragmentation and interface reconnection. The Lagrangian formulation cancels the interface diffusion, resulting in a sharp definition of interfaces between gas, liquid and structure. Moreover, SPH method can be applied to any continuum description, resulting in an ability to easily approach multi-physics. Therefore, SPH method can theoretically solve in a fully coupled way, the compressible multi-phase structural interaction problem occurring during impact phenomenon.

As the SPH method is best suited for fast dynamics, a careful attention need to be paid for slow dynamics like wave propagation. It would be completely inadequate to use the SPH method or any CFD software in order to simulate the propagation of a wave generated in a wave flume and then the impact phenomenon (complete problem). The propagation phase can be solved accurately by software based on potential theory (BEM for example), much faster than by CFD. However, such potential-theory-based software can obviously not simulate the local interactions between liquid, gas and structure that happen during impacts. Therefore, the strategy developed is based on a coupling between two codes sharing the different tasks. A potential-theory based code is in charge of the incident flow (non-perturbed wave train) and the SPH method is in charge of the local interactions simulations during the impact in the vicinity of the impacted structure. A specific forcing algorithm between potential solvers and SPH-flow was developed in order to reduce as much as possible the numerical diffusion of the wave trains between the wave generator and the structure. As a consequence, this method allows to simulate open sea problems, providing the incident wave field from a potential solution, and providing the fact that the diffracted wave field from the structure does not reflect on the inlet/outlet wave boundaries.

The paper is organized as follow: the different solvers used throughout the paper are presented. The coupling algorithm is explained and applied to a simple focused wave propagation case. The methodology is then applied to the simulation of greenwater events for a fixed simplified FLNG ship. Comparisons with experimental values are provided.

Modelling Sediment Resuspension in Industrial Tanks using SPH on GPUs

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***Abstract*—This paper presents a multi-phase model for frictional perfectly plastic sediment scouring induced by rapid flows. Attention is given to the fluid-sediment interface where sediment yielding is modelled using either the Mohr-Coulomb or the Drucker-Prager yield criterion for frictional materials. Post yield behaviour is modelled in a Newtonian approach by modifying the constitutive equations to include variable viscosity for the sediment phase. The model has been implemented on the GPU-based DualSPHysics code resulting in large computational speedup on the order of 45. Static and dynamic test cases have been modelled for both yield criteria to examine the interface, scouring intensity and post yield behaviour. Slight improvements were seen with the Drucker-Prager but correct prediction depends largely on the sediment material behaviour.**

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 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 producing a shear layer of suspended particles at the interface and finally sediment suspension in the fluid. To capture accurately complex industrial flows with variable physical properties for each phase, resolving small-scale effects at the interface is essential. GPU computing massively parallel architecture can dramatically accelerate simulations to feasibly simulate fine particle resolutions required for such industrial applications in realistic time.

In this study, a multi-phase fluid – sediment model based on two yield criteria, namely the Mohr-Coulomb and the Drucker-Prager have been implemented in DualSPHysics to model the scour and sediment suspension at the interface with attention to the viscous forces of the suspended sediment particles.

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 α and β denote the Cartesian coordinates using Einstein's summation and i and j the interpolated particle and its neighbours respectively.

A. Governinig Equations

The governing equations for density and momentum evolution of the field for the multi-phase model are given by [11]

$$\begin{cases} \dfrac{d\rho_i}{dt} = \rho_i \sum_j^N \dfrac{m_j}{\rho_j} u_{ij}^{\beta} \dfrac{\partial W_{ij}}{\partial x_i^{\beta}} \\ \dfrac{du_i^{\alpha}}{dt} = \sum_j^N m_j \left(\dfrac{\sigma_i^{\alpha\beta} + \sigma_j^{\alpha\beta}}{\rho_i \, \rho_j} \right) \dfrac{\partial W_{ij}}{\partial x_i^{\beta}} + g_i^{\alpha} \\ \dfrac{dx_i^{\alpha}}{dt} = u_i^{a} \end{cases}, \qquad (1)$$

where x_i^{α} is the position, u_i^{α} is the velocity, ρ is the density, $\sigma_i^{\alpha\beta}$ is the total stress tensor, m is the mass and g_i^{α} 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 [8]

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

where the viscous stresses are

$$\tau_i^{\alpha\beta} = 2\mu D_i^{'\alpha\beta}, \qquad (3)$$

and the deviatoric strain rate is defined as

GPU Acceleration of 3-D Multi-phase SPH Simulations for Violent Hydrodynamics

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***Abstract*—This paper investigates different programming algorithms for the acceleration of smoothed particle hydrodynamics (SPH) multi-phase simulations on graphics processing units (GPUs) using a modified version of the DualSPHysics code. The algorithms are tested with multiple particle resolutions using different test cases and different hardware. Four algorithms are proposed and their effect on the speedup of the multi-phase SPH GPU scheme is assessed using two different test cases: still water in a rectangular tank and a dam break simulation. The four different algorithms include conditional if-statements, conditional binary multipliers, separate particle lists and an intermediate CPU-GPU function. The results show that creating separate particle lists for different phases and their neighbours of each phase leads to approximately 10% speedup. Compared to a single-core CPU code, the speedup of the multi-phase GPU code is on the order of 40-80 depending on the GPU card being used. Finally, some initial results are presented for 3-D simulations for the SPHERIC benchmark test case of dam break impacting an obstacle.**

I. INTRODUCTION

Violent free-surface/hydrodynamic flows exist in various fields such as coastal and nuclear engineering. They include a diverse range of problems such as overturning waves and potentially explosive multi-phase pipe flow. However, due to the large nonlinear deformations and the rapid flow movement using a traditional Eulerian method such as finite volumes can be difficult because it requires a very fine, adaptive mesh. Lagrangian methods, which follow individual elements of the computational field and do not require a mesh, are more suitable in simulating violent flows.

SPH is a modelling method with extremely high computing requirements and its simulations require a substantial time period. This is due to the large number of calculations that are needed in order to simulate the interactions between the particles. Computing power is still not at the level where SPH simulations can be run quickly, especially when compared to methods such as finite elements or finite volume.

To perform convergence studies and to simulate industrial applications with SPH accurately, a large number of particles is needed. This is especially true with a multi-phase SPH scheme. The speed of sound in the two phases can differ enormously [1], creating an additional criterion for time integration. When modelling multi-phase flow the number of particles has naturally increased compared to the single-phase case. Considering for example a dam break test case, we not only need to simulate the moving water volume, but also the air volume around it. In three dimensions, the computational demands become even more severe with the number of particles required and the number of interactions.

To reduce the computational runtimes, two viable technologies exist: high-performance computing (HPC) and the use of graphics processing units (GPUs). Both technologies use parallel processing to accelerate simulations.

Graphics Processing Units (GPUs) are specialised hardware designed to process large quantities of data to be displayed on computer screens in real time. Primarily used for video games and image processing applications, their massively parallel architecture means they have emerged as a viable tool for scientific computing. Along with dedicated programming languages, such as CUDA (Compute Unified Device Architecture) and OpenCL (Open Computing Language), general purpose graphics processing units (GPGPUs) have recently emerged as a viable alternative to HPC due to lower purchase and maintenance costs. Creating a massively parallel HPC cluster, while effective, is a costly investment with large energy requirements.

The unique architecture of GPUs makes them particularly suitable for computationally intensive simulations using Lagrangian methods such as SPH. The large number of multi-processors on a GPU enables speed-ups close to two orders of magnitude compared to a single CPU code [2]. The first major computation of SPH using GPUs by Harada et al. [3] in 2007 used the texture memory, initially intended to store video game graphics for the particle attributes, constructing a data texture exclusively in the GPU. This avoided the memory transfer to the CPU which would significantly slow down the computation.

With the appearance of the CUDA compiler from nVidia GPU programming was made significantly easier. Despite their attraction for scientific computing, there has been only

SPH Modelling of Bed Erosion for Water/Soil-Interaction

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***Abstract*—The paper reports the development of a SPH based water/soil-interaction model and its application to different erosional dam-break flows. The novelty of the present approach refers to an attempt to harmonize an existing suspension model [13] with a critical bed-mobility condition to control the onset of the erosion process. The evolution of the liquid and granular phase particles is obtained from an SPH-integration of the continuity and momentum equations. The fluid is considered to be Newtonian. The soil-phase is modelled in line with a combined Hooke/Mohr-Coulomb approach. Depending on the ratio between the exerted viscous stress and the critical strength, particles which reside in the inner part of a fictitious suspension-layer are either assigned to a viscosity that is derived from a Chézy-relation between the shear stress and the local flow velocity, or associated to the underlying soil model. The water/soil-model has been implemented into the massively parallel hydrodynamic SPH code GADGET-H2O. Validation studies refer to the erosional dam-break experiments.**

I. Introduction

Water-induced soil erosion is a natural phenomenon frequently observed at soil beds of rivers and water ways but can also be caused by human activities, e.g. harbour-bed scours due to thrusters of manoeuvering ships. Investigations of water-induced soil erosion were usually performed experimentally in the past. Considering the experimental studies, attention should be paid to the very "classical" studies of Shields [9], who defined a stability parameter that explicitly tries to account for the critical shear-stress value above which a soil particle is considered to move. The original Shields-theory reveals some limitations: it holds under the very restrictive hypothesis of homogeneous non-cohesive soil and is confined to a horizontal bed slope. Subsequent studies were thus focused on a generalization of the classical theory to capture the influences of vegetation in natural channels and non-horizontal slopes [1].

More recently, water/soil-erosion studies were also carried out from a computational point of view, e.g. Manenti et al. [6], Roulund et al. [8] and Ulrich et al. [16]. Accordingly, Fraccarollo [5] and Spinewine et al. [10], [11] proposed a remarkable series of experimentally investigated dam-break cases, which can serve as benchmark cases for refined numerical water/soil-interaction models. They consists of a collapsing water column above a soil bed featuring different bed topographies, initial water heights and soil material. The related water/soil-flow is considered to be divided in three vertical layers with different characteristics. The lower layer is composed by solid material which is virtually at rest. It faces a centered mixture layer with an almost constant granular concentration and velocity. Finally an upper layer forms that is made of clear water moving with constant velocity. Grossly speaking, the lower layer behaves like a rigid body and the upper two layers are assumed to have a fluid-behaviour.

The SPH method represents a perfect candidate for the numerical investigation of water/soil-interaction problems. Related recent efforts were published by Ulrich et al. [13], [14], [15], [16], Manenti et al. [6] and Falappi et al. [4]. Former SPH results obtained from the present monolithic method by Ulrich et al. [13] generally displayed a fair representation of the fluid-soil interaction. No numerical distinction is made between the different layers – thus no stability criterion is used – and the vertical layers are identifed from the local values of the soil concentration. The goal of the present study is to introduce a stability condition into the model, and thereby control the initiation of the erosion process without compromising the model's general applicability. Accordingly, a critical shear stress derived from a Shields parameter is implemented in order to judge the mobility of particles. Depending on the ratio between the computed viscous stress and the critical stress, particles which reside in the (fictitious) suspension-layer are either associated with the underlying constitutive relations of the soil model or assigned to a viscosity derived from a Chézy relation. Model validations were performed against the aforementioned dam-break experiments of Fraccarollo et al. [5] and Spinewine [10].

The remainder of the paper is structured as follows: The SPH model is presented in the second section, while the third section is devoted to the investigated test cases. The fourth section displays the computed results. Conclusions are drawn in the fifth section.

II. SPH Computational Model

A. SPH Model basic structure

The employed SPH model [12] follows a classical approach and is therefore only described in brief. In the following, the subscript i indicates the focal particle, while j refers to neighboring particles found inside the kernel support. Greek

A pool boiling model with SPH

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***Abstract*—We present an SPH model of nuclear pool boiling in superheated liquid. We assume that heat supply via liquid phase is a rate limiting step for the phase change. Boiling model is defined on the particles level as follows. If an existing vapor particle has a temperature higher than T_s (saturation temperature) we insert a new vapor particle. To calculate heat flux over vapor-liquid interface (liquid-vapor particles interaction) we assume that all vapor particles have temperature T_s. So the heat flux over phase interface depends only on a temperature field in the liquid phase and does not depend on the temperature distribution in the vapor phase, which is distorted by release of latent heat during the evaporation. The other components of the model are Navier-Stokes equation for velocities, surface tension forces on the phase interface [1], and heat conduction [2].**

I. Introduction

Boiling can be a very efficient heat transfer mode for micro-devices. If fluid is allowed to boil in a channel it can remove up to ten times more heat for a given mass flow rate. Another advantages of boiling regime is fixed temperature of the phase transition which leads to a more predictable and uniform temperature field in the system [3]. But the applications of this phenomena into practice is still limited partially by the fact that there is a gap in understanding of the physics of transport phenomena in two-phase boiling flow in micro-channel. Nowadays many design decisions are made based on empirical correlations.

Physics in micro-channel can be qualitatively different from the macro-scale and it extrapolation of the results from macro- to micro-scale is not always justified. If system size changes from macro-scale to micro-scale the relative contribution of different physical phenomena is changing: importance of inertial and gravitational forces decreases, contribution of viscosity, surface tension, diffusion increases. Although the Reynolds number is small and inertia cannot be neglected and the solution of the full Navier-Stokes equations is required. The importance of surface tension requires accurate interface tracking and it is especially challenging in the present of phase change which may cause singularities and significant topological changes [4].

However, the number of experimental and modeling studies with aims to understand the physics of the boiling phenomena is rapidly growing. Experimental research is accelerated by application of high speed visualization techniques, and modeling is driving by faster computers and better simulations methods. In the following we outline the modeling works on nucleate boiling.

An analytical expression for single bubble growth in superheated liquid was obtained by Plesset and Zwick [5]. Fritz [6] gives prediction of bubble departure diameter from a heater surface based on static balance of buoyancy and surface tension forces. This results were extended to the dynamic regime by Mikic [7]. But application of analytical models is obviously limited to very simple situations and the first comprehensive numerical models were proposed by Welch [8] who used a moving mesh, two-dimensional finite volume method. After this pioneering work several numerical models were suggested.

Kunkelmann and Stephan [9] used the phase change model of Hardt and Wondra [10] in the Volume of Fluid (VOF) solver with a special treatment for the contact line evaporation [11]. Lee and Son [12] simulated nucleate boiling in micro-channel using level-set methods. Suh et al. [13] extended the method to simulate flow boiling in parallel microchannels. Mukherjee [14] combined level-set method with SIMPLER method. Hazi and Markus [15], applied lattice Boltzmann method and investigated heterogeneous boiling on a horizontal plate.

Several authors used particle-based models to simulate fluid-gas phase transition. Müller et al. [16] propose a technique to model boiling water with application to visualization. Yoon [17] used a combination of mesh-free methods (MPS-MAFL) for the calculation of nucleate pool boiling. A recent review of Koshizuka [18] is dedicated to applications of particle-based method in nuclear engineering and includes sections on heat transfer and boiling.

In this paper we use smoothed particle hydrodynamic (SPH) to simulate boiling in super-heated liquid. We solve the full NavierStokes equations and surface tension is modeled using method introduced by Hu and Adams [1].

II. Model

Our model consists of the following parts: momentum Navier-Stokes equations for velocity, surface tension forces on the interface between liquid and vapor phases, heat conduction, and evaporation model with supply of the heat as a rate limiting step.

A. Modeling of multi-phase flow in SPH

To model two-phase flow we use an approach from [1]. Here is a summary of equations solved. We consider Navier-Stokes

Application of Modified SPH to Quantum Mechanical Problems

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***Abstract*—We have applied Modified Smoothed Particle Hydrodynamics (MSPH) to quantum mechanical problems. The Schrödinger equation of a harmonic oscillator and the hydrogen atom are solved. The calculated results for MSPH are in good agreement with analytical solutions. The accuracy depends on the arrangement of the particles. To obtain high accuracy, many particles should be localized in the area where the wave function changes significantly. The results of using this method are also compared with those of the traditional finite difference method and the standard SPH. As a result, we have successfully shown that MSPH is efficient, and can therefore be applied to quantum mechanical problems with adequate accuracy.**

I. Introduction

Real-space calculation is quite an efficient way to investigate electronic structures, because the diagonal part of the Hamiltonian is dominant. It is widely used in recent state-of-the-art density functional theory [1]–[3], where the wave function is usually discretized by means of the finite difference (FD) method in a uniform mesh. In line with recent developments in the area of computer systems, this type of calculation is also suitable for large-scale parallel computing. However, a certain amount of calculation is still required in order to investigate electronic structures.

In large-scale calculation such as hydrodynamics analysis, on the other hand, Smoothed Particle Hydrodynamics (SPH) [4] is a typical meshfree particle method, and is very convenient and applicable for dealing with complex shapes, large deformations, and free surfaces. Currently, SPH is used in various fields for solving non-hydrodynamic partial differential equations such as the wave equation, Maxwell's equations, and Poisson's equation [5]–[7]. However, it lacks sufficient accuracy. To realize a similar level of accuracy, many more particles are necessary than mesh points in the FD method. Thus, it has not be evaluated sufficiently in quantum mechanical problems, because they require fairly high accuracy.

As a higher-accuracy method in an improved method of SPH, Modified Smoothed Particle Hydrodynamics (MSPH) [8], [9] has recently been developed. Although various improved versions of SPH have been proposed, it is reported that MSPH has higher accuracy than other versions [10]. In this paper, we have applied MSPH to several quantum mechanical problems. The Schrödinger equation of a harmonic oscillator and the hydrogen atom are solved. Since we can analytically obtain solutions for these problems, it is quite efficient to evaluate MSPH in quantum mechanical problems. The accuracy is compared to that of SPH and FD. First, we briefly review the SPH technique and then move on to an explanation of MSPH in quantum mechanical problems in Sec. II. In the following Sec. III, we discuss the results for a harmonic oscillator and hydrogen atom. Our conclusions are discussed in Sec. IV, and we summarize our findings in Sec V.

II. Methods

The one-dimensional Schrödinger equation is

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x)=E\psi(x)\ . \tag{1}$$

In the standard SPH picture, $\psi(x)$ and its second derivative are approximated as the following expressions [5];

$$\psi(x_i)\simeq\sum_{j=1}^{N}\psi(x_j)W_{ij}\frac{1}{n_j} \tag{2}$$

$$\left.\frac{\partial^2\psi}{\partial x^2}\right|_{x_i}\simeq\sum_{j=1}^{N}\psi(x_j)\frac{\partial^2 W_{ij}}{\partial x^2}\frac{1}{n_j}, \tag{3}$$

where

$$W_{ij}=W(x_i-x_j,h_{ij})=W(|x_i-x_j|,h_{ij}) \tag{4}$$

is the kernel and

$$n_i=\sum_{j=1}^{N}W_{ij} \tag{5}$$

is the particle number density. Through out this paper, we adopt the Gaussian type kernel function

$$W(r,h)=\frac{1}{h\sqrt{\pi}}\exp\left(-\frac{r^2}{h^2}\right), \tag{6}$$

and the smoothing length

$$h_{ij}=\frac{h_i+h_j}{2}. \tag{7}$$

Eq. (1) at the i-th particle position can be described

$$-\frac{1}{2}\sum_{j=1}^{N}\psi_j\frac{\partial^2 W_{ij}}{\partial x^2}\frac{1}{n_j}+V(x_i)\sum_{j=1}^{N}\psi_j W_{ij}\frac{1}{n_j}=E\sum_{j=1}^{N}\psi_j W_{ij}\frac{1}{n_j}. \tag{8}$$

Simulation of particulate suspensions with SPH and application to tape casting processes

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***Abstract*—The microscopic structure within the suspension during the tape casting process has a significant influence on the properties and quality of the final product. As it is often difficult to experimentally observe the behaviour of the particles in the suspension, a numerical model based on SPH has been developed which takes into account the hydrodynamics and the particle interactions. The model has been tested using the Jeffery orbit and applied to a suspension under shear load with different particle shapes.**

I. Introduction

Particulate suspensions play an important role in many industrial applications, such as ceramic processing, powder metallurgy, pharmaceutics or food processing. Often the microscopic structure within the suspension has a significant influence on the flow properties during processing and on the quality of the final product. Ceramic tapes produced by the tape casting process [1] often show an anisotropic shrinkage during the subsequent sintering process, which is directly related to the orientation of the non-spherical particles in the green tape [2]. This anisotropic orientation of the particles is related to the shear applied on the suspension during the tape casting process. This has already been numerically investigated on a macroscopic scale using the SPH method [3].

To be able to study the process on a microscopic level, the ceramic particles in the fluid must be modeled explicitly. Therefore, SPH particles are rigidly linked together in clusters in order to directly simulate the suspended particles in the fluid. The SPH method [4], [5] was extended by a rigid body solver governing the motion of these cluster. This allows for a straight-forward coupling between fluid and solid phase through the standard SPH interactions. As an advantage there are no constraints to the shape of the solid particles except those given by the resolution. The conjoint motion of the sub-particles is ensured by a rigid body propagation algorithm based on the quaternion approach described in [6], [7]. The idea of clustering sub-particles to model physical particles has also been used in other particle-based methods, e.g. the Discrete Element Method (DEM) [8], [9] and Dissipative Particle Dynamics (DPD) [10]. A similar SPH-based approach has been chosen by other groups [11], [12].

II. The tape casting process

Tape casting is a manufacturing process for thin ceramic tapes from a ceramic slurry. It consists of a continuously refilled reservoir of a cermic slurry with various organic additives underneath which a conveyor belt is used to produce a thin tape through the gap under the doctor blade (see Fig. 1). Often a second blade is used to dampen oscillations in the system caused by refilling the reservoir. Due to the movement of the conveyor belt and the hydrostatic pressure due to the slurry height in the reservoir a Couette flow superposed with a Poiseuille flows develops under the doctor blade. This shear applied on the slurry in this region has a major influence on the microstructure of the resulting ceramic tape.

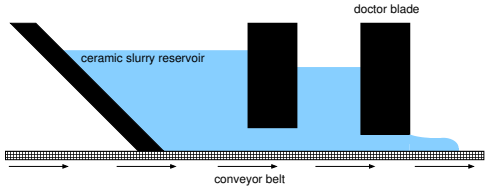

Fig. 1. Sketch of the principle constituents of a tape casting system

III. The model

In the following sections SPH-particles are always denoted "SPH-particles" and the physical particles are simply called particles or rigid bodies.

A. SPH Implementation

In the case of an incompressible, newtonian flow the governing equations for a fluid, the Navier-Stokes-equations, take the following form [13]

$$\frac{d\mathbf{v}}{dt} = -\sum_j m_j\left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right)\nabla W_{ij} + \sum_j m_j\left(\frac{\mathbf{T_i}}{\rho_i^2} + \frac{\mathbf{T_j}}{\rho_j^2}\right)\nabla W_{ij} \tag{1}$$

with $\mathbf{v}$ being the velocity of particle i (i=1 ... N, with N being the number of particles), m the mass and p the hydrostatic pressure. ρ is the density, $\mathbf{T}$ the viscous stress tensor at the location of the particles i and j. W_{ij} is the kernel interpolation function between particles i and j. A cubic spline is used as Kernel function [14]. The density is calculated through the summation formalism [14]

$$\rho_i = m_i \sum_j W_{ij}. \tag{2}$$

SmoothViz: An Interactive Visual Analysis System for SPH Data

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***Abstract*—The paper describes the software tool SmoothViz designed for visual representation and interactive analysis of data coming from SPH simulations with astrophysics as the driving application. Its main characteristics can be summarized as follows: (1) All visualization methods operate directly on particle data, i.e., any kind of re-sampling or regularization of the original data is avoided. (2) The system supports the analysis of individual scalar and vector fields as well as a simultaneous analysis of multiple fields. (3) The system works with time-varying volumetric physical spaces and respective attribute spaces, where each attribute refers to a field. (4) Interactive analysis is supported by the use of multiple coordinated views, i.e., a number of views of different properties of the data are provided. When the user interacts with one view (e.g., by making a selection) the interactions are immediately reflected in all other views (e.g., by highlighting the selection in all views).**

I. Introduction

Since its invention by Gingold and Monaghan [1] and Lucy [2], SPH simulations produce datasets of permanently increasing size. They involve millions of particles and operate with tens of scalar and vector fields. Data may include thousands consequent time steps of a simulation. Thus, there is a clear need for systems assisting the researchers in exploring such complex datasets. Visualization methods provide intuitive means for data representation, which form a basis for interactive data exploration and analysis. We introduce our system SmoothViz which is targeted at interactive visual analysis of unstructured multi-variate time-dependent volumetric data.

Interactivity when running SmoothViz on an off-the-shelf PC is achieved by means of multi-processor (OpenMP) and GPGPU (CUDA) implementations of the main algorithms, including isosurface extraction, stream- and pathlines tracking, scatterplot generation, etc. The user has access to the information at different levels of abstraction (e.g., particle parameters or characteristics of selected groups) in a textual or visual form. The first main view of the graphical user interface (GUI) of SmoothViz (implemented in Qt) is a 3D physical space visualization widget (implemented in OpenGL) allowing the user to explore individual scalar and vector fields, the range of influence of individual particles, etc. To analyze the multidimensional attribute space of multi-field data, a linear projection method is used in the frame of a star-coordinate widget, which allows the user to understand the attribute values of the particles. It facilitates the intuitive detection of groups of particles with similar characteristics and behavior.

Designed for visual analysis and representation of SPH astrophysical data, SmoothViz can be applied to SPH data from other fields and even to non-SPH point-based unstructured data. In the latter case, Moving Least Squares (MLS) technique is used instead of the standard SPH approximation formula. MLS is able to approximate both values of the sampled field and its derivatives of arbitrary order [3]–[6] with prescribed smoothness degree.

II. Related Work

Several visualization tools exist to work with SPH data, e.g., SPLASH [7], which serves to visualize one-, two- and three-dimensional SPH results consistently with the basic SPH method. SmoothViz was first introduced by Linsen et al. [8] and has been incrementally extended to include state-of-the-art visualization algorithms and developed according to the user feedbacks.

An SPH vector field visualization technique based on a predictor-corrector scheme was proposed by Schindler et al. [9]. The authors were able to extract smooth vortex core lines using the native SPH interpolation procedure.

One of the most popular scalar field visualization approaches is the generation of isosurfaces, i.e., manifolds at which the considered scalar field takes a given value. Isosurface extraction from unstructured point-based volume data was in the focus of papers by Rosenthal and Linsen [10], [11]. These approaches are incorporated in the SmoothViz system.

Since the simulated data typically contain a multitude of physical variables, their interplay is an important part of data analysis. A simple but efficient approach is to investigate the

$\langle MPS \rangle \equiv \langle SPH \rangle$

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***Abstract*—The consistency of Moving Particle Semi-implicit (MPS) method in reproducing the gradient, divergence and Laplacian differential operators is discussed in the present paper. Its relation to the Smoothed Particle Hydrodynamics (SPH) method is rigorously established. The application of the MPS method to solve the Navier-Stokes equations using a fractional step approach is treated, unveiling inconsistency problems when solving the Poisson equation for the pressure that are exemplified with one dimensional simple cases. Some corrections to these issues are outlined and a brief discussion on incompressible SPH links with MPS is provided.**

I. Introduction

The "Moving Particle Semi-implicit" method (MPS) is a numerical technique first introduced by Koshizuka and Oka in the nineties [1], [2] to solve incompressible Navier-Stokes equations. It relies on a meshless discretization of the continuum to approximate differential operators. In order for the obtained flow field to exhibit the properties of an incompressible flow, a fractional time step approach is used. This approach requires solving a Poisson equation for the pressure field at every time step, which consequently demands a numerical approximation of the Laplacian operator.

Similarly to SPH, the MPS scheme is mainly used to solve violent free-surface flows, exploiting the fact that no mesh is needed for the computations [3]–[5]. Regardless all that body of work neither the derivation of the MPS numerical method from its first principles, nor its consistency in regards to how accurately it reproduces the continuum as the numerical resolution increases, have been discussed at length in the literature. As CFD practitioners we believe this issue is paramount in order to guarantee the Engineering applicability of the numerical technique.

The present paper addresses this matter by first analyzing the consistency of the MPS approximations to the gradient, divergence and Laplacian operators and deriving continuous integral forms of these approximations. Second, the connections with SPH are rigorously presented by relating, through the integral form of the operators, the MPS weighting function with the SPH kernel. Third, the integral form of the operators is applied to the solution of the Poisson equation used in MPS for the pressure computation through the fractional step methodology. Some problematic issues regarding the implementation of Dirichlet and Neumann boundary conditions are discussed and exemplified with one dimensional simple cases. Finally, some corrections to these issues are outlined and a brief discussion on incompressible SPH links with MPS is provided.

II. Governing equations

Newtonian incompressible flows are the ones treated with the MPS method. The incompressible Navier-Stokes equations in Lagrangian formalism are hence taken as the field equations:

$$\frac{D\mathbf{r}}{Dt} = \mathbf{u}, \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{2}$$

$$\frac{D\mathbf{u}}{Dt} = \mathbf{g} + \frac{\nabla\cdot\mathbb{T}}{\rho}. \tag{3}$$

where ρ stands for the fluid density and $\mathbf{g}$ is a generic external volumetric force field. The flow velocity $\mathbf{u}$ is defined as the material derivative of a fluid particle with position $\mathbf{r}$. $\mathbb{T}$ denotes the stress tensor of a Newtonian incompressible fluid:

$$\mathbb{T} = -P\boldsymbol{I} + 2\mu\mathbb{D}, \tag{4}$$

in which P is the pressure, $\mathbb{D}$ is the rate of deformation tensor ($\mathbb{D} = (\nabla\mathbf{u} + \nabla\mathbf{u}^T)/2$) and μ is the dynamic viscosity. With this notation, the divergence of the stress tensor $\mathbb{T}$ is computed as:

$$\nabla\cdot\mathbb{T} = -\nabla P + \mu\nabla^2\mathbf{u}. \tag{5}$$

MPS is based on a Helmholtz-Hodge decomposition of an intermediate velocity field initially devised by Chorin [6] in the late sixties. First, an intermediate velocity field $\mathbf{u}^*$ is explicitly computed using the momentum equation but ignoring the pressure term. Second, the zero divergence condition is imposed on the velocity field at the next time step, thus obtaining the Poisson equation for the pressure:

$$\nabla^2 P = \frac{\rho}{\Delta t}(\nabla\cdot\mathbf{u}^*), \tag{6}$$

in which Δt is the time step. Once the pressure is found, pressure gradients and particle positions are modified. A comprehensive flow-chart of the whole approach can be found in e.g. [7].

III. MPS discretization

A. Density and number density

The set of equations (1-3) has to be discretized in order to implement the fractional step algorithm. The fluid domain is discretized in a set of particles and the differential operators at an individual particle i are evaluated using the value of the different fields at the neighboring particles. The MPS method weights these neighboring particle properties by using a compactly supported function w whose argument is the distance between particles $\left|\mathbf{x}_i - \mathbf{x}_j\right|$ normalized with the cut-off radius r_e and which is non-negative. The weighting function is

A transport-velocity formulation for Smoothed Particle Hydrodynamics

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***Abstract*—The tensile instability of the standard weakly-compressible SPH method implies a serious limitation for high Reynolds number flows that occur in many real applications. In this work the problem of particle clumping and void regions in a flow caused by negative pressure is solved with a modification of the particle advection velocity. The basic concept to use a modified velocity for the position change of a particle was used already before (e.g. Xu et al. [1]), but we propose a new method to obtain this advection velocity and derive an effective stress term for the momentum conservation [2]. Still, the presented method is exactly conservative and does not need any parameter calibration. We have applied our method to a wide range of test cases and found unprecedented accuracy and stability.**

I. Introduction

In this work we propose a new transport-velocity formulation for weakly-compressible SPH that resolves an important dilemma of the classical WCSPH scheme. According to the theory of incompressible flow, the pressure in the fluid takes effect merely by its gradient. Therefore, the flow is invariant of a superimposed constant background pressure field, i.e. it is gauge invariant. However, since the standard SPH is not 0th-order consistent, gauge invariance is not recovered numerically, leading to a spurious pressure gradient from a formally constant pressure field. Hence, the simulation results change with different background pressures. Ideally, no background pressure should need to be added to the system. On the other hand, when a low (zero) background pressure is imposed, SPH suffers from the so-called tensile instability. This instability is caused by particle clumping due to attraction forces between neighboring particles with effectively negative pressures. A possible solution to this problem is to increase the background pressure that ensures non-negative pressures in the entire domain, but as mentioned before this introduces additional numerical viscous dissipation that can be comparable to the physical viscous dissipation. Thus, increasing the background pressure effectively changes the Reynolds number of the flow, and consequently the application of SPH to practical industrial applications is substantially impeded. Note that our method mainly addresses the tensile instability problem, a ”cousin of the pairing instability” with the same symptoms [3]. As a side-effect we found that with the new method the pairing instability [4] does not occur either. Alternatively the latter instability could also be circumvented by using kernels that have non-negative kernel Fourier transforms [3], [5].

In 1989 Monaghan [6] addressed the problem of penetration in particle methods and proposed a modified advection velocity based on a smoothing of the velocity field. This so-called XSPH correction can improve the smoothness of the flow field, but, strictly speaking, the smoothing is arbitrary involving an unknown parameter. Another classical workaround for the clumping problem is to use an artificial viscosity that stops particles approaching each other when they are very close, e.g. Monaghan [7]. Whilst this artificial dissipation can be shown to take effect as a physical viscosity, and thus is used to simulate real flows at finite Reynolds numbers, at the same time the numerical dissipation required to stabilize the simulation of high Reynolds number flows can become comparable to the physical viscosity and of course strongly affects the results.

For truly incompressible SPH methods the particle clumping problem is easily suppressed as the divergence-free condition for the velocity field and the constant-density condition can be enforced separately. Hu and Adams [8] use a fractional time-step integration with an intermediate projection step and experienced no problems with particle penetration. Xu et al. [9] proposed an ISPH method that takes advantage of an additional diffusion-based particle shifting scheme ensuring well homogenized particle configurations at all times. Very recently, Lind et al. [10] extended this approach for free-surface problems where the standard method failed due to the incomplete kernel support of particles at the free surface. Additionally, they use the kernel gradient normalization and approximate the shifted particle quantities by a Taylor series to improve the accuracy of the scheme.

As a new, fundamentally different approach, we present here a simple and effective algorithm based on the classical WCSPH without need for additional parameters and involving only a marginally small computational overhead. The new method is characterized by the different utilization of a background pressure on computing the particle momentum velocity and the particle advection velocity. As a consequence of the new advection velocity, an additional term appears in the momentum equation that accounts for the difference between the motion of a particle and its averaged momentum.

SPH simulations of elastic turbulence and mixing in a periodic channel flow

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***Abstract*—Using SPH simulations of a viscoelastic fluid modelled with an Oldroyd-B constitutive equation, we demonstrate that the flow through a closely-spaced linear array of cylinders confined in a channel undergoes a transition to a purely elastic turbulent regime above a critical Weissenberg number (We). The high-We regime is characterized by an unsteady motion and a sudden increase in the flow resistance in qualitative agreement with experimental observations. Furthermore, a power-law scaling behavior of the integral quantities as well as enhanced mixing of mass is observed. A stability analysis based on the Dynamic Mode Decomposition method (DMD) allows us to identify the most energetic modes responsible of the unsteady behavior which correspond to filamental structures of polymer over/under-extension advected by the main flow preserving their shape. These time-dependent flow features resemble strictly the *elastic-waves* reported in recent numerical simulations.**

I. Introduction

Elastic turbulence represents an intriguing phenomenon occurring in complex flows of polymer solutions and corresponding to the onset of a randomly fluctuating fluid motion even in the creeping flow limit, at vanishing Reynolds number. Although the study of elastic instabilities in complex fluids dates back to the early 90's [1], [2], it was not until the seminal paper of Steinberg and Groisman [3] that a complex global flow motion was experimentally observed and the term "*elastic turbulence*"coined. Although there is no common agreement on the definition of "turbulence", the term was introduced by [4] due to the identification of strong similarities in the phenomenology observed in the flow of polymer suspensions with those commonly characterizing ordinary hydrodynamic turbulence, namely: (i) significant increase in flow resistance, (ii) randomly fluctuating fluid motion with fluctuations increasing with the liquid elasticity, (iii) broad continuum range of temporal/spatial frequencies involved, with power-law spectral scaling behavior, (iv) enhanced mixing of mass. Based on these analogies, the work of [4] shows that elasticity-induced turbulence could be obtained through a moderate increase in the We number. In such conditions the flow is characterized by features which are comparable to those observed in hydrodynamic turbulence for Re numbers of around 10^4.

In this article we report evidence of purely elastic instability and transition to turbulence and mixing in a wall-bounded periodic flow geometry characterized by a linear array of cylinders confined in a channel. This flow geometry and the corresponding unbounded one (square array of cylinders) have been widely investigated in the past, both experimentally and numerically, with controversial results. In particular, the unbounded case has been investigated experimentally in [5]–[8] where elastic instabilities were generally observed to show up together with a modification of the global flow behavior: as a critical Weissenberg number is achieved, flow quantities start to exhibit fluctuations which increase in magnitude as the effect of liquid elasticity becomes more pronounced. Moreover, this phenomenon is accompanied by an abrupt increase in the flow resistance which is believed to be related to a non-linear transition from a steady state towards a more dissipative time-dependent flow structure [7]. Less effort has been devoted in the past to the experimental study of the corresponding wall-bounded geometry, nevertheless analogous flow features have been reported in the literature [8], [9]. Although the wall-bounded two-dimensional flow was experimentally [9] and numerically [10] found to be unstable to three-dimensional perturbations at a given critical Weissenberg number, to date no numerical method has been able to predict either the unsteady behavior or the large abrupt drag increase observed in experiments. In [11], two-dimensional Lagrangian simulations using a particle method (Smoothed Particle Hydrodynamics) allowed to observe the transition mentioned above at a critical Weissenberg number of $O(1)$, significantly smaller than the one considered to be the threshold for the onset of three-dimensional flow (~ 1.55). In this article, we perform a detailed investigation of the flow transition process using the Dynamic Mode Decomposition (DMD) approach recently developed in [12]. DMD is a technique that allows for a modal analysis of a data sequence, without resorting to a numerical solver or an underlying model [12]. In the case of a linearized flow (i.e. a flow of small perturbation about a steady base flow), the extracted structures are equivalent to global eigenmodes. For a nonlinear flow, the decomposition produces modes that express the dominant dynamic behavior captured in the

Simulating 3D turbulence with SPH

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***Abstract*—In this paper, we have investigated the ability of Smoothed Particle Hydrodynamics (SPH) to simulate turbulent flows. It is well known that the standard method without corrections cannot predict the energy cascade of a turbulent flow. In the absence of viscosity, standard SPH simulations become divergent and at finite viscosities the method overpredicts dissipation. As a remedy, we have introduced a modified transport velocity to advect particles that homogenizes the particle distribution, thus stabilizes the numerical scheme. In addition, artificial dissipation is strongly reduced and we successfully applied the new method to transitional flows. Here, we present two- and threedimensional simulation results of the Taylor-Green vortex flow. We analyzed the energy spectra and dissipation rates and found good agreement with DNS data from literature.**

I. Introduction

Presented independently by [Lucy(1977)] and [Gingold & Monaghan(1977)], Smoothed Particle Hydrodynamics (SPH) was first introduced with the aim of simulating astrophysical problems where its grid-less nature is obviously advantageous. But over the years, SPH was successfully applied to many other fields ranging from structural mechanics to complex multi-phase flows with transport models of surface active agents [Monaghan(2005)], [Adami *et al.*(2010)].

Turbulence modeling with SPH is still a rather new area of research. The difficulty of the standard method for this application is two-fold. On one hand, in the absence of physical viscosity, i.e. when solving the Euler equations with SPH, by the nature of the method conservation of energy implies negligible numerical dissipation that finally drives the flow to a randomly fluctuating system. On the other hand, when solving the Navier-Stokes equation at finite Reynolds number, the non-gauge free property of the pressure-term discretization in conservative form introduces additional numerical dissipation that can be comparable to the physical viscous dissipation and damp the flow excessively.

In 2002 Monaghan [Monaghan(2002)] showed a Lagrangian averaged Navier-Stokes turbulence model-type modification of the original SPH method and simulated two-dimensional turbulence. Although achieving good results, this method was shown to be computationally very inefficient [Mansour(2007)]. [Violeau & Issa(2007)] presented three different turbulence models for SPH, two algebraic models and one based on the Reynolds Stress Model. They applied their method to 2D open channel turbulent flows and 2D collapsing water column and could improve the quality of the benchmark results compared to the original SPH. But compared to state-of-the-art results with a grid-based method the comparison was still poor. [Dalrymple & Rogers(2006)] simulated two-dimensional breaking waves with SPH using a LES-type turbulence model. [Robinson & Monaghan(2012)] and [Mansour(2007)] studied how well SPH performs in a Direct Numerical Simulation (DNS). They show that the original SPH method can reproduce the (inverse) energy cascade but their work is still limited to two-dimensional problems. [Ellero *et al.*(2010)Ellero, Español & Adams] and [Shi *et al.*(2012)] showed that SPH in its original form has effectively an implicit viscosity and shows some characteristics of turbulent flows when applied to high Mach number, isentropic homogeneous flows.

In this work we present a novel SPH method to simulate turbulent flows. Based on the standard SPH formulation [Monaghan(2005)], [Hu & Adams(2006)] we introduce a transport velocity different from the momentum velocity to advect particles. This fundamental modification was first proposed by [Monaghan(1989)], who used a kernel-based smoothing of the flow field to advect particles and showed that his *XSPH* method is very similar to a Lagrangian averaged Navier-Stokes turbulence model [Chen *et al.*(1998)Chen, Foias, Holm, Olson, Titi & Wynne], [Holm(1999)]. Different from XSPH, we solve a modified momentum equation including a constant background pressure field that regularizes particle motion "physically" while strongly reducing artificial numerical dissipation. Details of this method are given in the next section and our two- and three-dimensional results show that SPH is capable of simulating turbulent flows.

II. Numerical method

In this section we briefly introduce the governing equations for a Newtonian fluid and introduce briefly the SPH framework.

A. Governing equations

The isothermal Navier-Stokes equations are solved in a Lagrangian frame of reference. Thus, mass conservation gives

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\mathbf{v}\ , \tag{1}$$

where ρ is the density of the fluid and $\mathbf{v}$ is the velocity vector. In the absence of body forces, the momentum equation reads

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{v}\ . \tag{2}$$

Dynamic Load Balancing for SPH

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***Abstract*—We evaluate the performance of different load balancing algorithms used in the open source SPH framework PySPH. We focus on algorithms that are used to generate particle decompositions that adapt to the dynamic nature of the simulation as opposed to spatial domain decomposition methods. A synthetic test case for particles randomly distributed in a box and the (2D) dam break problem with an obstacle are used as test cases to measure the efficiency of the algorithms and quality of the partitions. The relatively simple geometric algorithms are found to perform well in this context with the Recursive Inertial Bisection (RIB) method producing the best partitions for the problems considered.**

I. Introduction

Smoothed Particle Hydrodynamics (SPH) is a meshless method employing the use of points/particles as discretization entities for the numerical simulation of continuum mechanics problems. The governing PDEs are transformed into ordinary differential equations for particle field variables, constraining individual particles to interact with near neighbors. The subsequent motion of particles with the local material velocity renders the method Lagrangian. As a numerical tool, SPH is a competitive option for large deformation problems in arbitrary domains for problems in astrophysics, solid-mechanics and incompressible fluid flow [1]–[3]. The principle application area of SPH remains free surface flows in which an incompressible fluid moves under the influence of gravity in an open vessel [4]–[6]. In comparison to mesh based methods, SPH is characterized by requiring a large number of entities (particles) for an accurate description of the flow and more computations per entity than their mesh based counterparts. Furthermore, the explicit nature of most SPH implementations imply stringent time step criteria for stability which further increases the computational time required. In these circumstances, one must look for parallel paradigms for any realistic SPH implementation. The choice for parallelism is complicated by the vast array of available hardware ranging from clusters to hybrid computing environments that leverage the processing power of massively parallel graphics processing hardware (GPUs) [7]. In general, parallel implementations can be categorized as data or task parallel. Domain decomposition falls into the data parallel model wherein the particles are distributed across available processors in a distributed computing environment. The processor assignment can either be spatial according to the domain or adapt to the particle distribution. In this work, we focus on the class of decomposition algorithms that adaptively re-distribute particles in an arbitrary domain. Specifically, we discuss the class of geometric load balancing algorithms that rely on coordinate bisection, space filling curves or a k-means clustering approach. Although the discussion on load balancing is application agnostic, we use the 2D dam break problem in the presence of an obstacle as a concrete test case. The choice of this problem is justified considering that the problem adds a sufficient amount of complexity like multiple species (fluid, solid) and boundary conditions without obfuscating the parallel implementation with the details of the SPH algorithm. More generally, the discussion in this work is applicable to any dynamic simulation with short range particle interactions. We work within the framework of PySPH and use the Zoltan data management library [8], [9] for the bisection and space filling curve partitioners. The algorithms are assessed on the execution times and quality of partitions in terms of the number of particles exchanged per iteration.

The outline of the paper is as follows. In Sec. II, we describe the parallel algorithm for distributed memory machines we adopt for PySPH. We briefly describe some of the load balancing algorithms applicable to SPH in Sec. III before going on to discuss the results for the algorithms implemented for the box test and a dam break problem with an obstacle in Sec IV. Finally, we summarize and conclude this work in Sec. V.

II. Smooth Particle Hydrodynamics

We outline a typical sequence of SPH operations for a problem and the parallel model for the implementation adopted in PySPH. The basic assumption for the model is a distributed memory machine equipped with the message passing library (MPI).

A. Serial SPH

SPH can be introduced via the theory of kernel interpolation whereby a sufficiently smooth function f can be approximated at an arbitrary point $\boldsymbol{x}$ in a domain Ω by summing contributions from near-neighbors

$$f(\boldsymbol{x}) \approx \sum_{b \in \mathcal{N}(\boldsymbol{x})} f_b W(|\boldsymbol{x} - \boldsymbol{x}_b|, h) \Delta_b \tag{1}$$

The interpretation is that the function values are weighted by a kernel function W, and Δ_b is the nodal volume associated with an interpolation point. The kernel is compactly supported

Effective memory layout and accesses for the SPH method on the GPU

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***Abstract*—The smoothed particle hydrodynamics (SPH) method has been implemented on Graphical Processing Units (GPU) several times to increase performance. However, the need for ever faster implementations is still there. Modern GPUs have a complex memory hierarchy of which effective utilization is paramount for high-performance computing. Use of the GPU's shared memory has traditionally been seen as important, as GPUs have had no or little automatic caching. Newer GPUs from NVIDIA, such as the Fermi and Kepler architectures, have a more advanced cache implementation than previous generations, possibly alleviating the shared memory requirement. We present benchmark results of four different memory handling strategies for the SPH algorithm with computations on the GPUs and with kernel support width of both $2h$ and $3h$. Our results indicate that modern caching to a great extent alleviate the need for explicit and manual use of shared memory, and that the kernel support has a great influence on the choice of memory strategy.**

I. Introduction

The smoothed particle hydrodynamics (SPH) method [1] was first used in astrophysics in the late 1970s, though since the 1990s it has seen widespread use in simulation of weakly compressible fluids [2]. As SPH-simulations are computationally very expensive, it is natural to deploy them on graphical processing units (GPU) that provide high-floating point throughput in a cost effective manner.

In this paper we first give an overview of related work that perform SPH computations on massively parallel hardware. In Section III we give a short introduction to the computational aspects of the SPH method, as well as an introduction to the core concepts of GPU programming. In Section IV we sketch our implementation and describe various memory fetching strategies. Penultimately we present our numerical experiments, and report report on the observed performance for different number of particles and kernel support widths in SectionV.

We conclude and make a comparison between the achieved and theoretical maximum performance on the GPU used in Section VI. Finally, to aid in reproducibility we give a detailed description of the various algorithms in Appendix A.

II. Related work

The first full GPU implementation of the SPH method was introduced by Harada et al in 2007, see [3], using an OpenGL based implementation.

In 2010 Goswami et al [4] presented an interactive CUDA implementation with surface extraction and rendering. Their implementation uses shared memory for caching of particle data as well as Z-ordering of indices for coalesced optimal reads.

Recently the open-source SPHysics simulator [5] was extended to DualSPHysics which added GPU acceleration through CUDA, an overview of this process is described in [6].

III. Background

In this section we recap the SPH-method and GPU-computing concepts to define a common terminology used throughout our work. It is not intended as a full introduction to either of them.

A. An introduction to the SPH method

We briefly describe the SPH method in this section, for a smoother introduction, please consult [1], [2], [7]. We shall only consider the three dimensional case, though the exposition can be easily extended to n dimensional case without difficulty.

In the SPH method a medium of fluid is approximated using a finite set of *particles*, each with its own position, velocity, density, pressure, mass and possibly other properties which will not be described here. Formally the particles are represented as finite sets of time-dependent functions $\{\mathbf{r}_i\} \subset C^\infty(\mathbb{R}, \mathbb{R}^3)$, $\{\mathbf{v}_i\} \subset C^\infty(\mathbb{R}, \mathbb{R}^3)$, $\{p_i\} \subset C^\infty(\mathbb{R}, \mathbb{R})$ and $\{\varrho_i\} \subset C^\infty(\mathbb{R}, \mathbb{R})$ denoting the position, velocity, pressure and density for each point in time, i.e. the velocity of particle i at time t is $\mathbf{v}_i(t)$. When the point in time is clear, we will often omit the time argument and abuse notation by $f_i(t) = f_i$.

Following standard notation, we shall let $w_h : \mathbb{R}^3 \to \mathbb{R}$ be a smoothing function, as described in e.g. [7], where $h \in \mathbb{R}$ is a smoothing factor. Functions $f : \mathbb{R}^3 \to \mathbb{R}$ are replaced by a discrete approximation, $\hat{f}(\mathbf{x}) = \sum_i V_i f(\mathbf{x}_i) w_h(\mathbf{x} - \mathbf{x}_i)$.

Efficient Massive Parallelisation for Incompressible Smoothed Particle Hydrodynamics with 10^8 Particles

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***Abstract*—The incompressible smoothed particle hydrodynamics (ISPH) method with projection based pressure correction has been shown to be highly accurate and stable for internal flows. This paper describes an alternative parallel approach for domain decomposition and dynamic load balancing by using Hilbert space filling curve to decompose the cells with number of particles in each cell as the cells' weight functions. This approach can distribute particles evenly to MPI partitions without losing spatial locality which is critical for neighbour list searching. As a trade-off, the subdomain shapes become irregular. The unstructured communication mechanism has also been introduced to deal with halo exchange. Solving sparse linear equations for pressure Poisson equation is one of the most time consuming parts in ISPH using standard preconditioners and solvers from PETSc[1]. The particles are reordered so that insertions of values to the global matrix become local operations without incurring extra communications, which also have the benefit of reducing the bandwidth of coefficients matrix. The performance analysis and results showed the promising parallel efficiency.**

I. Introduction

Smoothed Particle Hydrodynamics(SPH) codes have been effectively parallelised using domain decomposition methods, implemented with libraries such as MPI for a long time. However, to efficiently maintain geometric locality of particles within processors and deal with dynamic load balancing arising from solving a complex, highly nonlinear and distorted flow is still hot topic. The highly scalable parallel performance relies on a good assignment of particles to processors and grouping physically close particles within a single processor reduces inter-processor communication.

There are several domain decomposition techniques used by the various existing MPI-based SPH fluid simulation models, The standard block partition method has been employed by SPhysics, DualSPhysics [1], which is easy to use, but handles poorly load balancing issues arising from solving highly complex, nonlinear and distorted flow.

[1]PETSc: http://www-unix.mcs.anl.gov/petsc/petsc-2/index.html

The particles' irregular distribution and complex-shaped computational domain prevent using the traditional simple domain decomposition methods with large number of particles due to load balancing issues. PPM [2] and SPH-Flow [3] have a implementation of Recursive Orthogonal Bisection, (ROB), In the ROB algorithm, the computational domain is first divided into two regions by a cutting plane orthogonal to one of the coordinate axes so that half the work load is in each of the sub-regions. The splitting direction is determined by computing in which coordinate direction the set of objects is most elongated, based upon the geometric locations of the objects. The sub-regions are then further divided by recursive application of the same splitting algorithm until the number of sub-regions equals the number of processors. However, the ROB method does not generally produce very fine granularity load balancing since it is based on cutting with a hyperplane.

This paper describes an alternative partitioning and dynamic load balancing approach by using Hilbert Space Filling Curve (HSFC) to decompose the cells with number of particles in each cell as the cells' weight functions. Comparing with ROB, this approach is less demanding computationally than ROB [4] and can distribute particles evenly to MPI partitions with fine granularity, and avoids losing spatial locality which is critical for neighbour list searching. As a trade-off, the subdomain shapes become irregular. The unstructured communication mechanism has also been introduced to deal with halo exchange.

Solving sparse linear equations for the pressure Poisson equation is one of the most time consuming parts in ISPH. The ISPH code uses standard preconditioners and solvers from PETSc. The particles are reordered so that insertions of values to global matrix become local operations without incurring extra communications, which also have a benefit of reducing the bandwidth of coefficients matrix.

This paper is organised as follows, Section II introduces the basic ISPH equations. Then sections III and IV describes the domain decomposition method and dynamic load balancing